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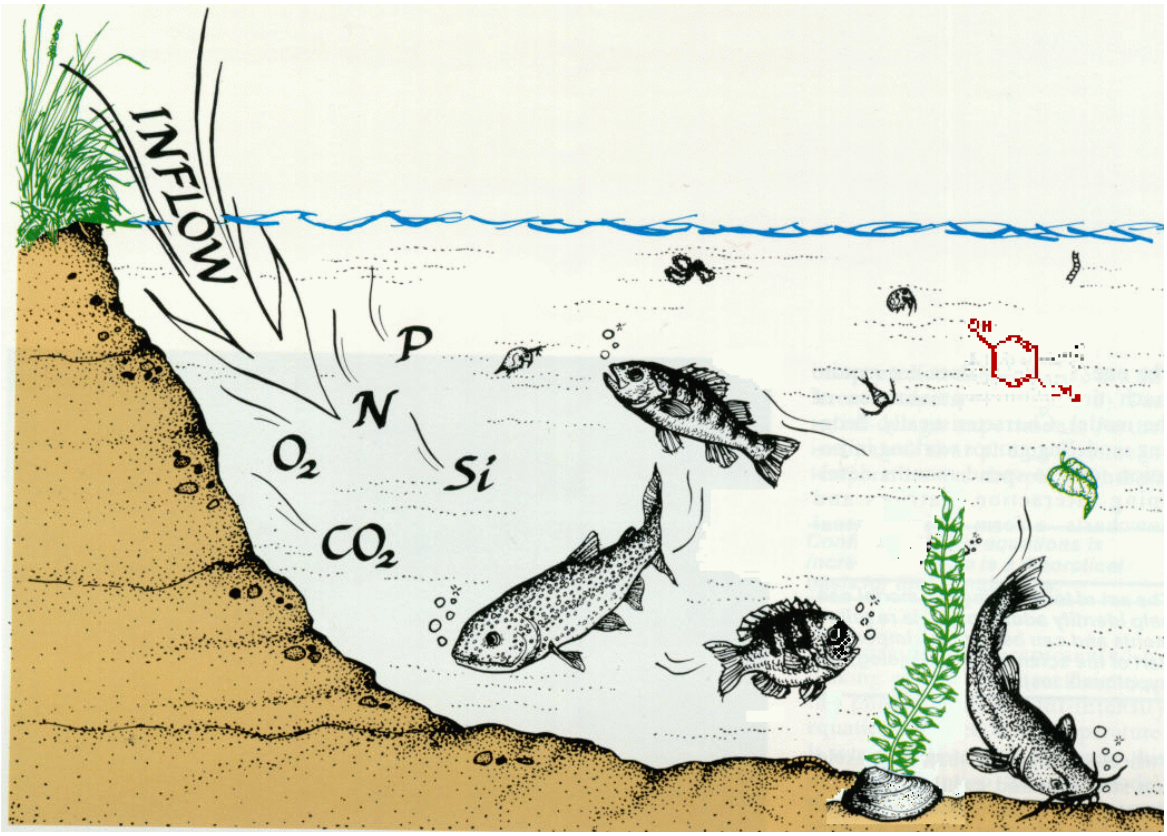
AQUATOX FOR WINDOWS

A MODULAR FATE AND EFFECTS MODEL FOR AQUATIC ECOSYSTEMS

RELEASE 1

VOLUME 1: USER'S MANUAL



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VOLUME 1: USER'S MANUAL

SEPTEMBER 2000

U.S. ENVIRONMENTAL PROTECTION AGENCY
OFFICE OF WATER
OFFICE OF SCIENCE AND TECHNOLOGY
WASHINGTON DC 20460

DISCLAIMER

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This document describes a new aquatic ecosystem simulation model. It is not intended to serve as guidance or regulation, nor is the use of this model in any way required. This document cannot impose legally binding requirements on EPA, States, Tribes, or the regulated community.

ACKNOWLEDGMENTS

This model has been developed and documented by Dr. Richard A. Park of Eco Modeling; most of the programming has been by Jonathan S. Clough under subcontract to Eco Modeling. It was funded with Federal funds from the U.S. Environmental Protection Agency, Office of Science and Technology under contract number 68-C4-0051 to The Cadmus Group, Inc. Work assignment managers for The Cadmus Group have been Paul Jacobson, Jonathan Butcher, and William Warren-Hicks; their help in expediting the contractual arrangements and in reviewing the scientific approaches is appreciated. Revision of the documentation has been performed under subcontract to AQUA TERRA Consultants, Anthony Donigian, Work Assignment Manager, under EPA Contract 68-C-98-010.

Additional Federal funding for program development has come from the U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, through Purchase Orders 7W-0227-NASA and 7W-4330-NALX to Eco Modeling.

The assistance, advice, and comments of the EPA work assignment manager, Marjorie Coombs Wellman of the Exposure Assessment Branch, Office of Science and Technology has been of great value in developing this model and preparing this report. Further technical and financial support from David A. Mauriello and Rufus Morison of the Office of Pollution Prevention and Toxics is gratefully acknowledged.

In an earlier version of the model developed at Abt Associates, Brad Firlie facilitated the programming; Rodolfo Camacho developed and programmed the inorganic sediment constructs; and review was provided by Lisa Akeson, Elizabeth Fechner-Levy, and Keith Sappington.

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PREFACE

The Clean Water Act— formally the Federal Water Pollution Control Act Amendments of 1972 (Public Law 92-50), and subsequent amendments in 1977, 1979, 1980, 1981, 1983, and 1987— calls for the identification, control, and prevention of pollution of the nation's waters. In the National Water Quality Inventory: 1996 Report to Congress, 36 percent of assessed river lengths and 39 percent of assessed lake areas were impaired for one or more of their designated uses (US EPA 1998). The most commonly reported causes of impairment in rivers and streams were siltation, nutrients, bacteria, oxygen-depleting substances, and pesticides; in lakes and reservoirs the causes also included metals and noxious aquatic plants. The most commonly reported sources of impairment were agriculture, nonpoint sources, municipal point sources, atmospheric deposition, hydrologic modification, habitat alteration and resource extraction. There were 2196 fish consumption advisories, which may include outright bans, in 47 States, the District of Columbia and American Samoa. Seventy-six percent of the advisories were due to mercury, with the rest due to PCBs, chlordane, dioxin, and DDT (US EPA 1998). States are not required to report fish kills for the National Inventory; however, available information for 1992 indicated 1620 incidents in 43 States, of which 930 were attributed to pollution, particularly oxygen-depleting substances, pesticides, manure, oil and gas, chlorine, and ammonia.

New approaches and tools, including appropriate technical guidance documents, are needed to facilitate ecosystem analyses of watersheds as required by the Clean Water Act. In particular, there is a pressing need for refinement and release of an ecological risk methodology that addresses the direct, indirect, and synergistic effects of nutrients, metals, toxic organic chemicals, and non-chemical stressors on aquatic ecosystems, including streams, rivers, lakes, and estuaries.

The ecosystem model AQUATOX is one of the few general ecological risk models that represents the combined environmental fate and effects of toxic chemicals. The model also represents conventional pollutants, such as nutrients and sediments, and considers several trophic levels, including attached and planktonic algae, submerged aquatic vegetation, several types of invertebrates, and several types of fish. It has been implemented for streams, small rivers, ponds, lakes, and reservoirs.

The AQUATOX model is described in these documents. **Volume 1: User's Manual** describes the usage of the model. Because the model is menu-driven and runs under Microsoft Windows on microcomputers, it is user-friendly and little guidance is required. Volume 2: Technical Documentation provides detailed documentation of the concepts and constructs of the model so that its suitability for given applications can be determined. Volume 3: Model Validation Reports presents three model validation studies performed for different environmental stressors and in different waterbody types.

1. QUICK START

1.1 System Requirements

Minimum Requirements

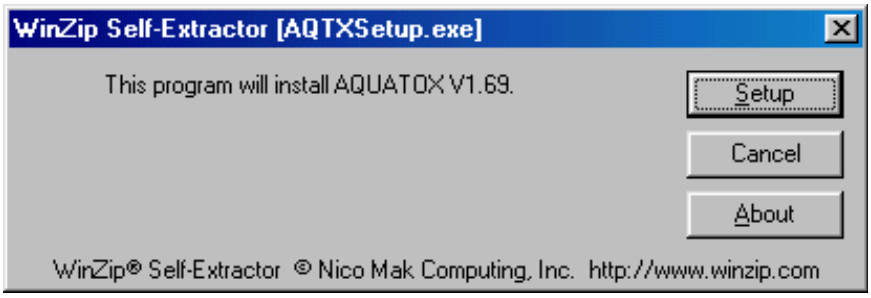
- PC Compatible, Intel 486DX 66 MHz
- Microsoft Windows 95, 98, or NT
- 16 MB RAM
- 30 MB free disk space

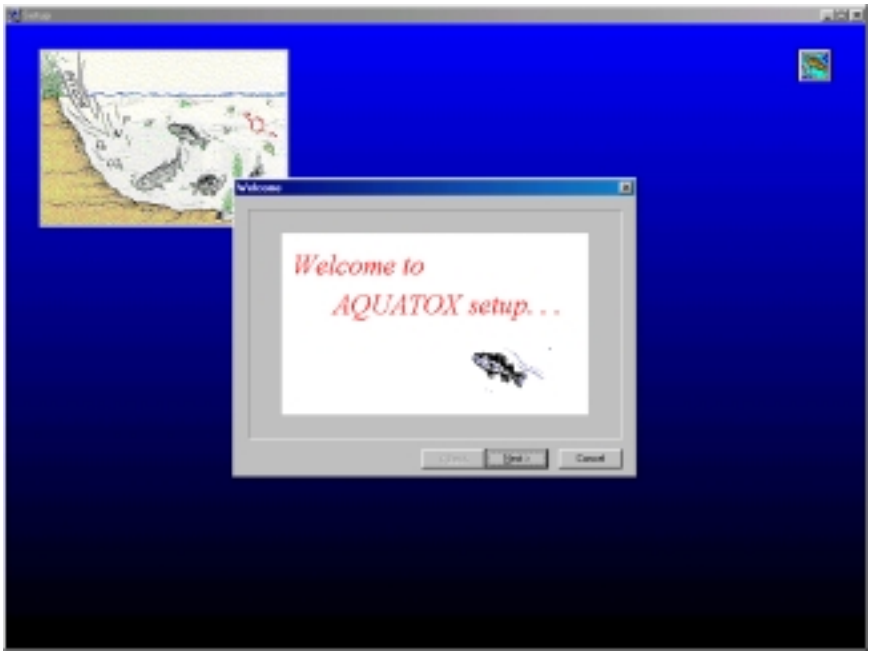
Recommended

- Pentium PC, 300 MHz or higher
- 64 MB RAM
- 75 MB free disk space

1.2 Installation

To install AQUATOX, run AQTXSetup.exe, the files will unzip, and InstallShield will lead you through the straightforward installation.

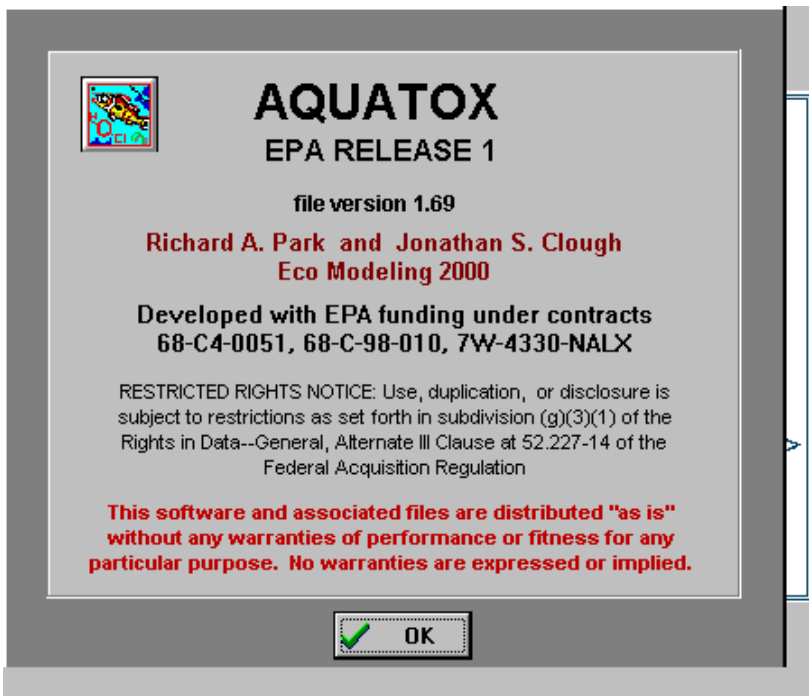




1.3 Starting

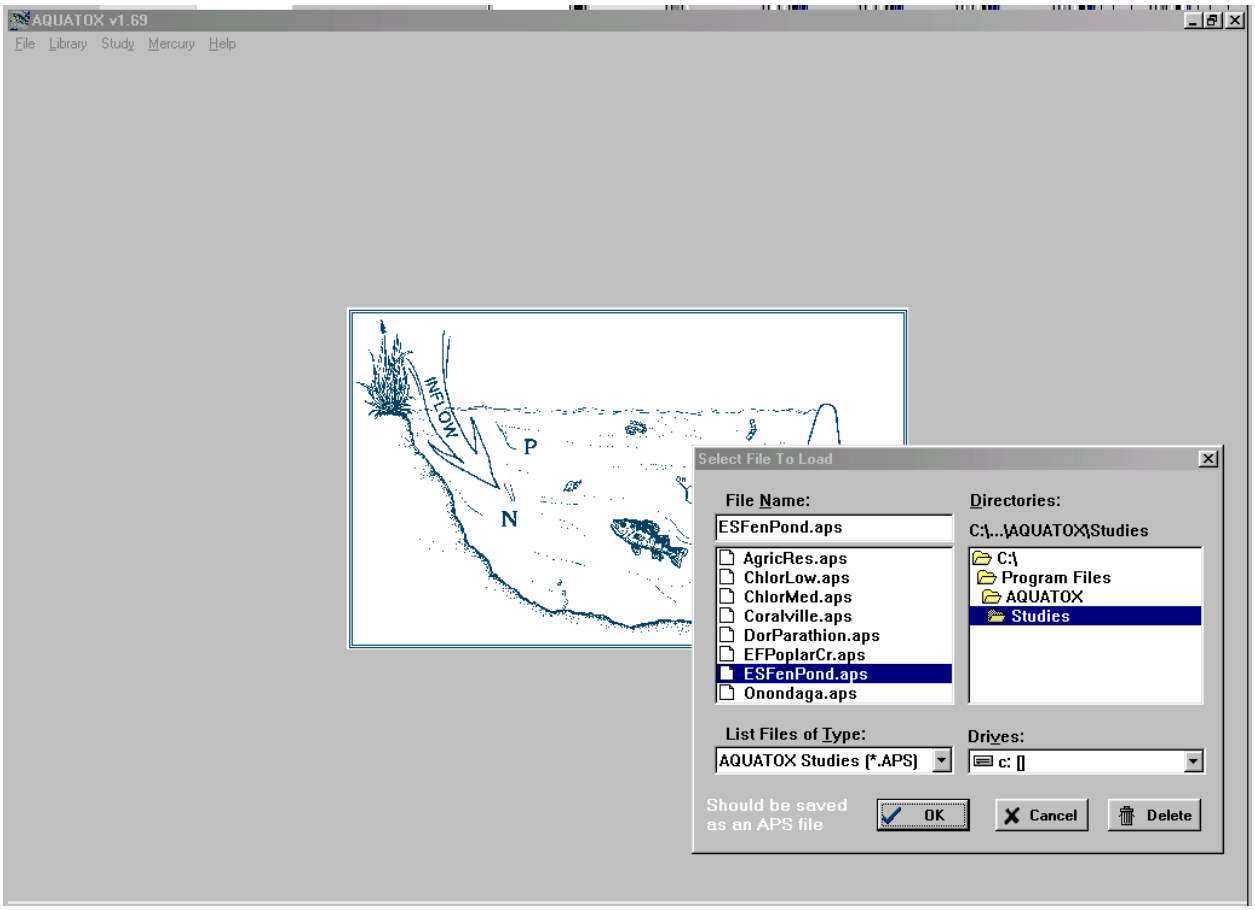
Double-click on the AQUATOX icon in Windows to open the program.

Then a "splash" window will open briefly, indicating that the model is still subject to modification and that, while the model is in the public domain, there are parts of the model interface that are proprietary.

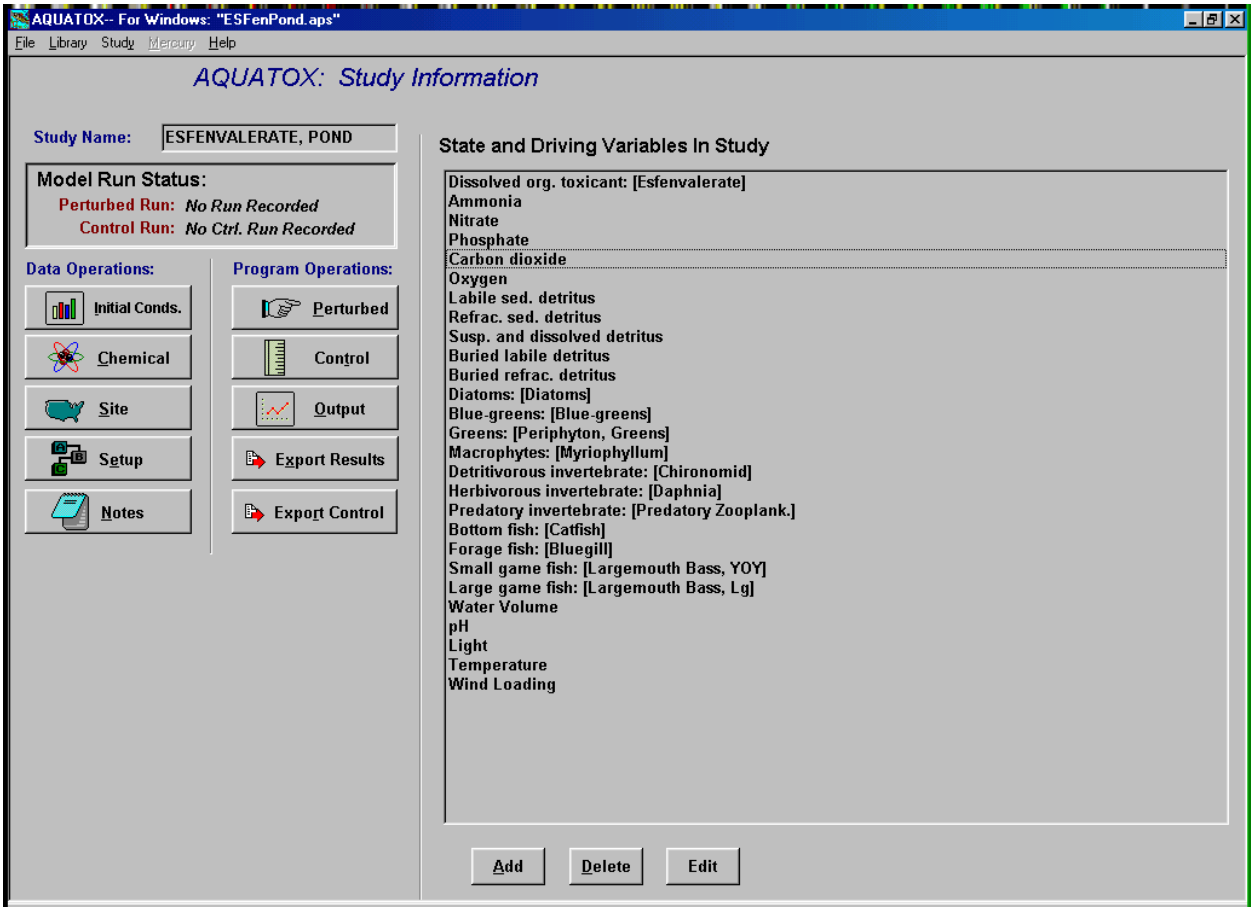


1.4 Loading a Study

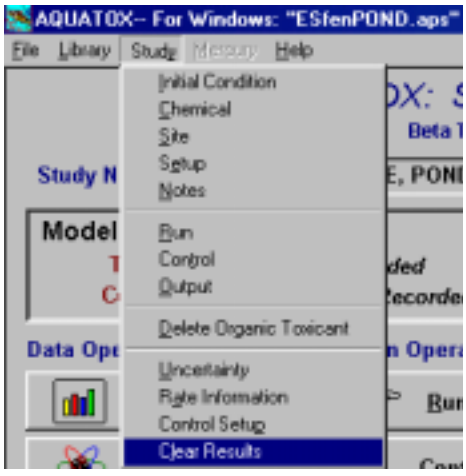
The study is the basic unit in AQUATOX; it contains site data, loadings, and parameter values used in a simulation; and it may contain results from a prior simulation. Usually we model one study at a time; however, there is a batch mode that is described later. Click on **File** in the menu bar to get the pull-down file menu, and click on **Open**. You will then be given a choice of AQUATOX study files to load. For this example we will choose **Esfenpond.aps**.



The main window will appear with the name of the study, the list of state variables used, and buttons from which to choose various operations. The **Study Name** can be edited; it is separate from the name of the file, which you loaded and which is displayed at the top of the screen. The study name is used as a title in graphical output, so is best capitalized. The **Status** window tells when the perturbed and control runs were made, and warns if they are incomplete or outdated. The **Initial Conditions** button brings up a screen with all the state variable values at the beginning of a simulation. The **Chemical** button brings up the parameter screen for the organic toxicant, if modeled. Double clicking on **Dissolved org. toxicant** at the top of the list of state variables and driving variables has the same effect. The **Site** button loads the site characteristic screen. **Setup** allows the user to set the dates of the simulation, and to specify various options such as the control setup, uncertainty analysis, and saving biologic rates. **Notes** provides a window for writing comments on the study. **Perturbed** starts the simulation with changed conditions, such as with a toxicant. **Control** starts a simulation without the stressor; the user can use **Control Setup** as mentioned above to specify what is changed and what is held constant. **Output** presents the results as a series of charts and graphs. The output can be exported as database files by clicking on **Export Results** or **Export Control**. **Help** is not yet implemented, except the **About** window, which brings up the splash window.



To save a file, click on **File** then **Save** or **Save As** on the menu bar; you will also be given an opportunity to save an altered file before exiting or loading another file. Study files range in size from 25 KB to over 2 MB. If you wish to minimize the size of a study—for example, to transmit to someone else—you can strip out the results by clicking on **Study** and choosing **Clear Results** from the menu bar. The study files distributed with AQUATOX have been minimized in this way.

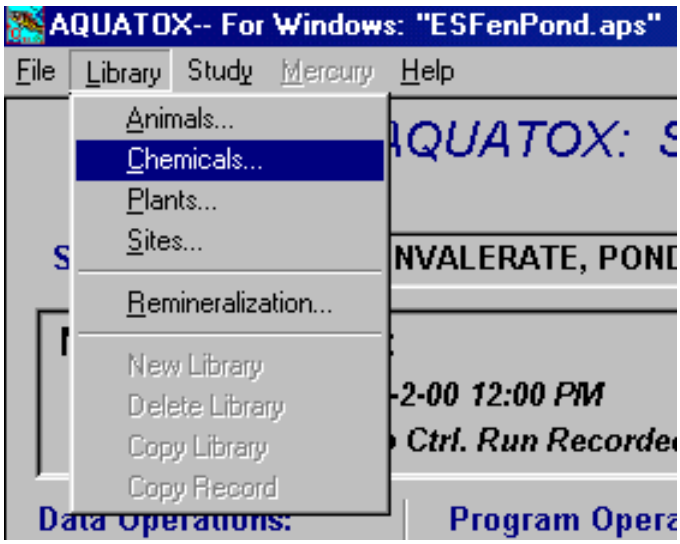


1.5 Loading a Library

There is a basic dichotomy in working with AQUATOX. You have a choice of editing database files in the general library or of opening a particular study. Studies are self-contained files with all the information on a particular simulation, including initial conditions, loadings, parameter values, first and last dates for the simulation, and simulation results. Parameter values can be edited, but changes apply *only* to that study. The intent is to be able to archive a model application so that all assumptions and results are saved for future reference. This is especially important for regulatory applications that are subject to later review. (Of course, you also should archive the version of AQUATOX that was used.)

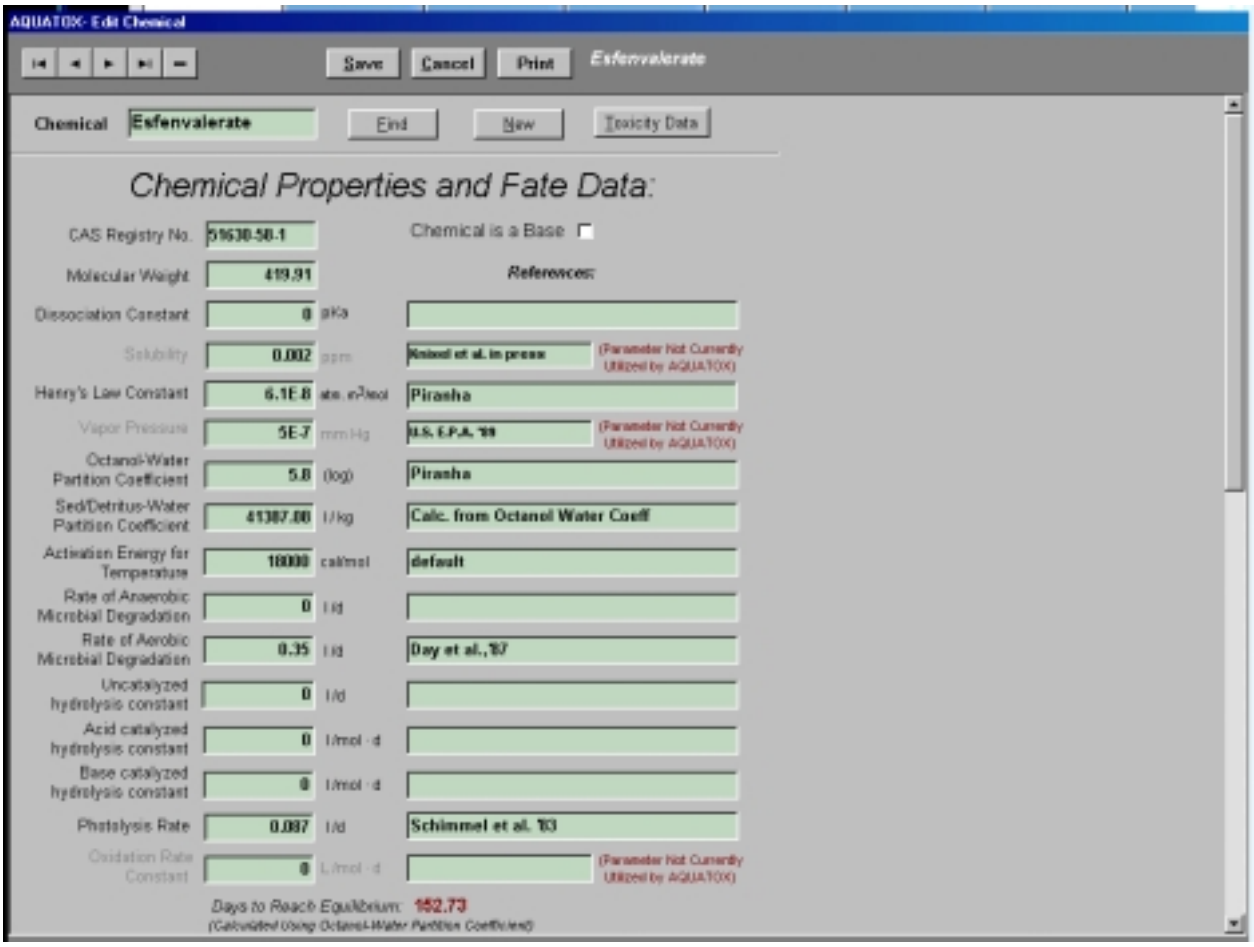
Parameter and site records that will be used repeatedly should be saved in the appropriate library. Each library is a database in Paradox format with records for each organism, chemical, or site. Generally, editing of parameters should be done in the library mode to maintain consistency among studies. In contrast, if a site record is only going to be used for a single study, it may be desirable to create it within the study. Study records can be copied into the library; so the choice of where to edit parameters is up to the user. It is the user's responsibility, though, to synchronize parameter values among studies. This can be done by saving a record to a library and then loading that record to each study.

To create or edit a record for general use, click on **Library** in the menu bar. You can then click on the specific library from the pull-down menu.

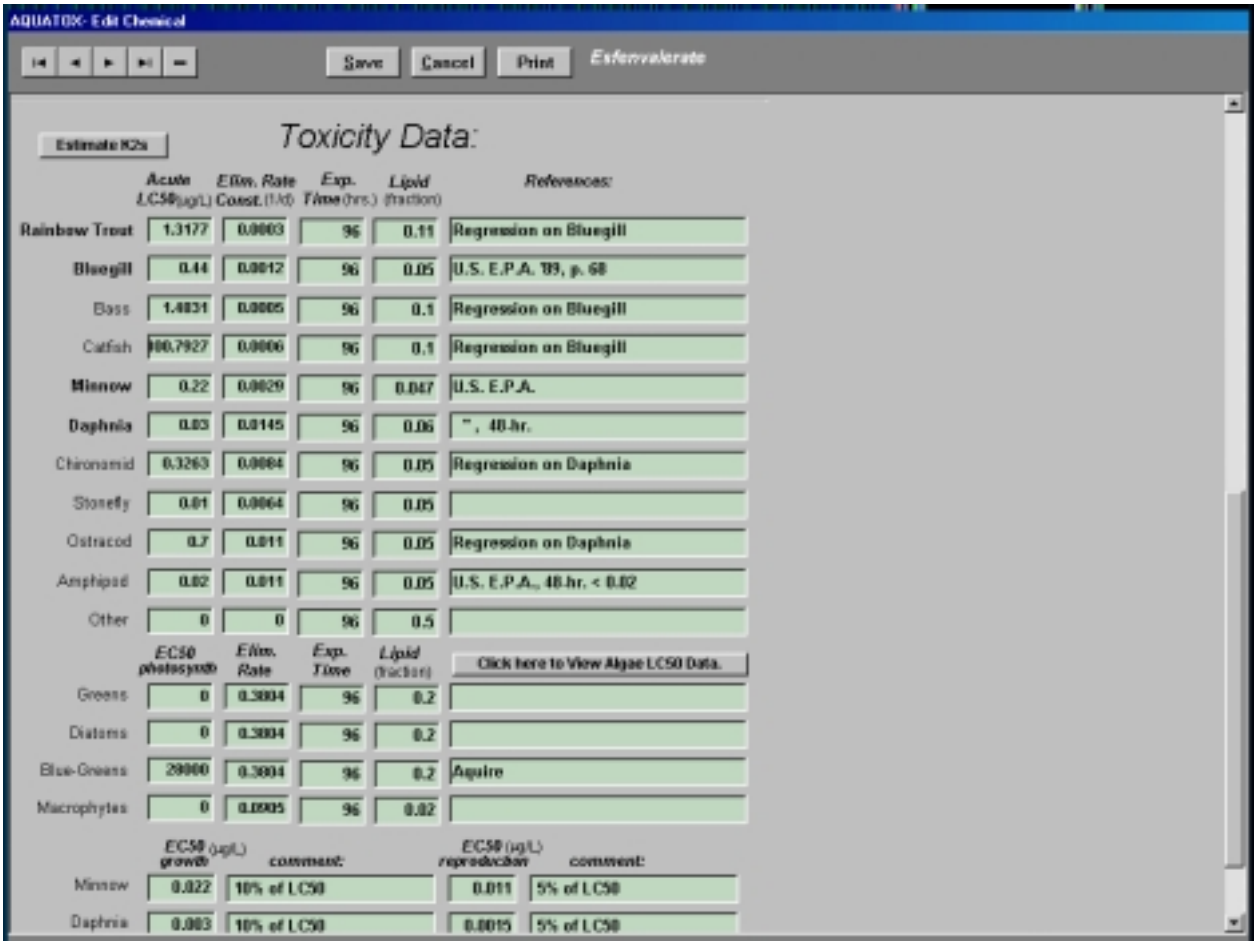


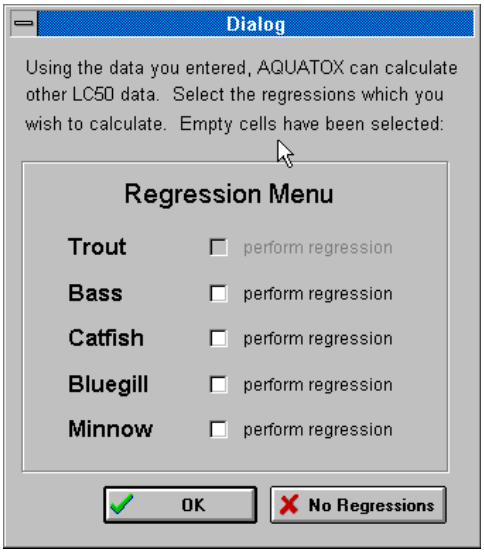
In this example we will choose **Chemical** and **Default** in sequence. The first record is for atrazine. We can click on the arrows in the upper left or can search for a particular name to move through the database. Use the arrow to move to Esfenvalerate. When you leave a database you will be asked whether you want to save it or lose any changes you might have made. The frequent requests for confirmation may be irritating, but they are for your protection. Any time you leave a record you may back out of a change by not saving it. There is no undo capability, so if you save a change, you are stuck with it, except by re-editing the entire record. It is easy to print a record, and you are

encouraged to make a hard copy before you make extensive changes. Some variables are not used at this time and are so indicated.



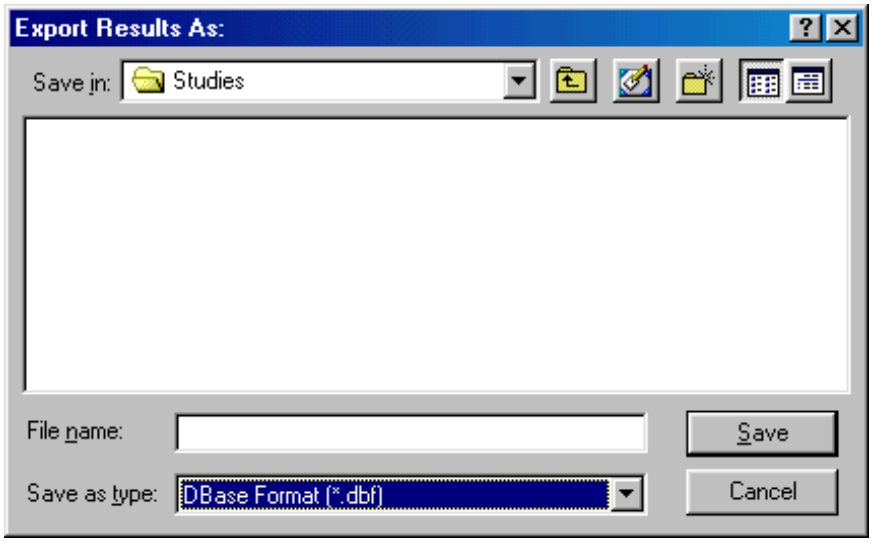
You can see the lower part of the screen, which gives toxicity data for the chemical, by clicking on the scroll bar at the right or by clicking on the **Toxicity Data** button at the top right. Toxicity can be estimated for several organisms, given data for others indicated in bold type. For example, change the LC_{50} for trout from 1.3177 to 1.4 (or any other value). You will then get a window presenting you with other organisms for which the LC_{50} can be estimated. If any have zero values, they will be checked automatically. The estimation procedures were developed with pesticide databases (Mayer and Ellersieck, 1986, Suter et al., 1986), so they should be applied with caution to industrial chemicals.


AQUATOX- Edit Chemical
Save
Cancel
Print
Esfenvalerate
Estimate K2s
Toxicity Data:
Acute LC50 (µg/L)
Elim. Rate Const. (1/d)
Exp. Time (hrs.)
Lipid (fraction)
References:
Rainbow Trout 1.3177 0.0003 96 0.11 Regression on Bluegill
Bluegill 0.44 0.0012 96 0.05 U.S. E.P.A. '89, p. 68
Bass 1.4831 0.0005 96 0.1 Regression on Bluegill
Catfish 100.7927 0.0006 96 0.1 Regression on Bluegill
Minnow 0.22 0.0029 96 0.047 U.S. E.P.A.
Daphnia 0.03 0.0145 96 0.06 ", 48-hr.
Chironomid 0.3263 0.0004 96 0.05 Regression on Daphnia
Stonefly 0.01 0.0064 96 0.05
Ostracod 0.7 0.011 96 0.05 Regression on Daphnia
Amphipod 0.02 0.011 96 0.05 U.S. E.P.A., 48-hr. < 0.02
Other 0 0 96 0.5
EC50 photosynth
Elim. Rate
Exp. Time
Lipid (fraction)
Click here to View Algae LC50 Data.
Greens 0 0.3804 96 0.2
Diatoms 0 0.3804 96 0.2
Blue-Greens 28000 0.3804 96 0.2 Aquire
Macrophytes 0 0.0005 96 0.02
EC50 growth (µg/L)
comment:
EC50 reproduction (µg/L)
comment:
Minnow 0.022 10% of LC50 0.011 5% of LC50
Daphnia 0.003 10% of LC50 0.0015 5% of LC50


Dialog
Using the data you entered, AQUATOX can calculate other LC50 data. Select the regressions which you wish to calculate. Empty cells have been selected:
Regression Menu
Trout perform regression
Bass perform regression
Catfish perform regression
Bluegill perform regression
Minnow perform regression
OK
No Regressions

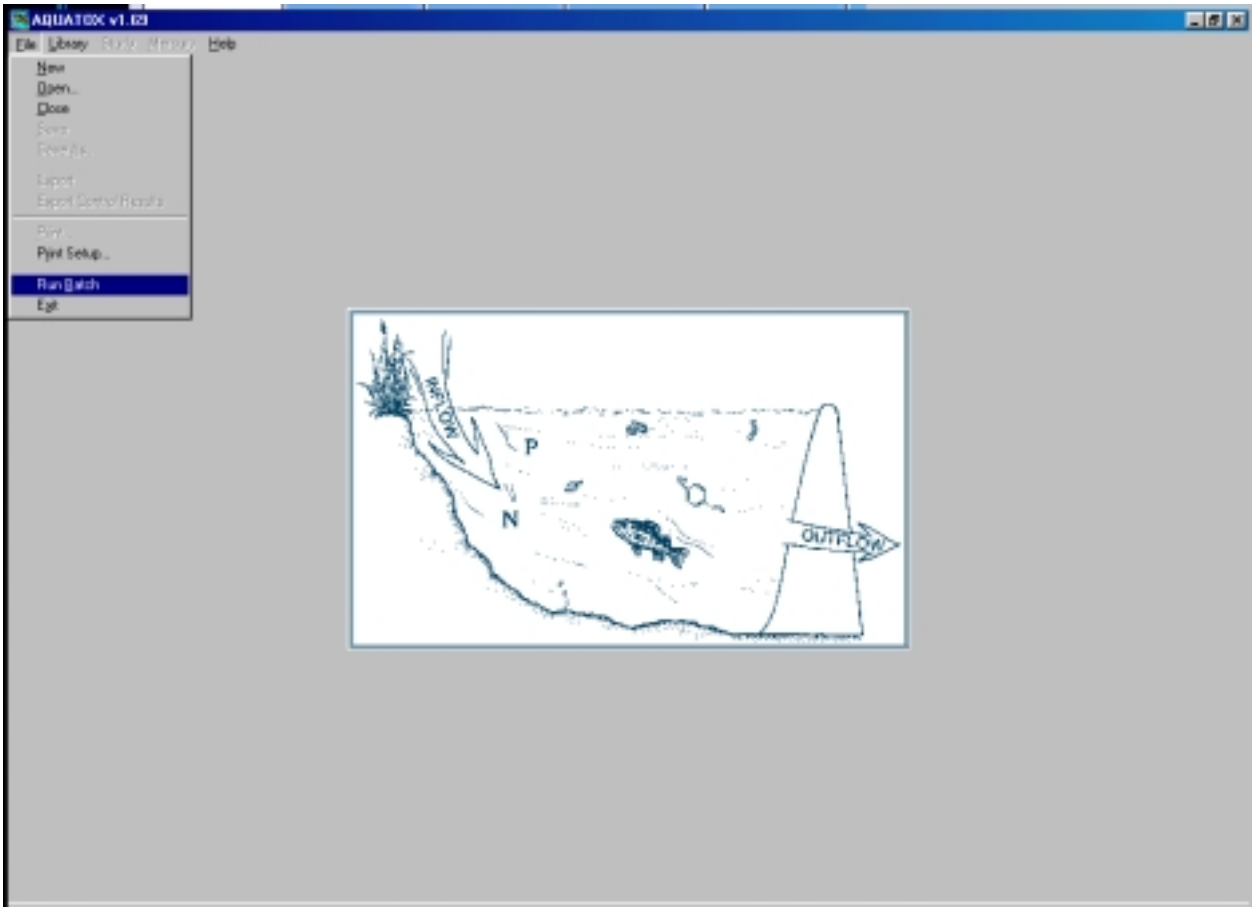
1.6 Running and Saving a Simulation

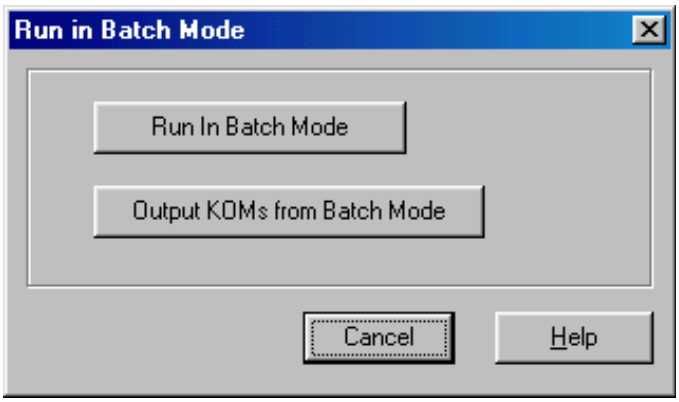
You can run both **Perturbed** and **Control** simulations to see the impacts of various stressors. The results can be exported in dBase, Paradox, or text (Prn) formats. When you click on **Export** you will be given the Study subdirectory as the default for saving the results; you may wish to choose the Output or some other directory.

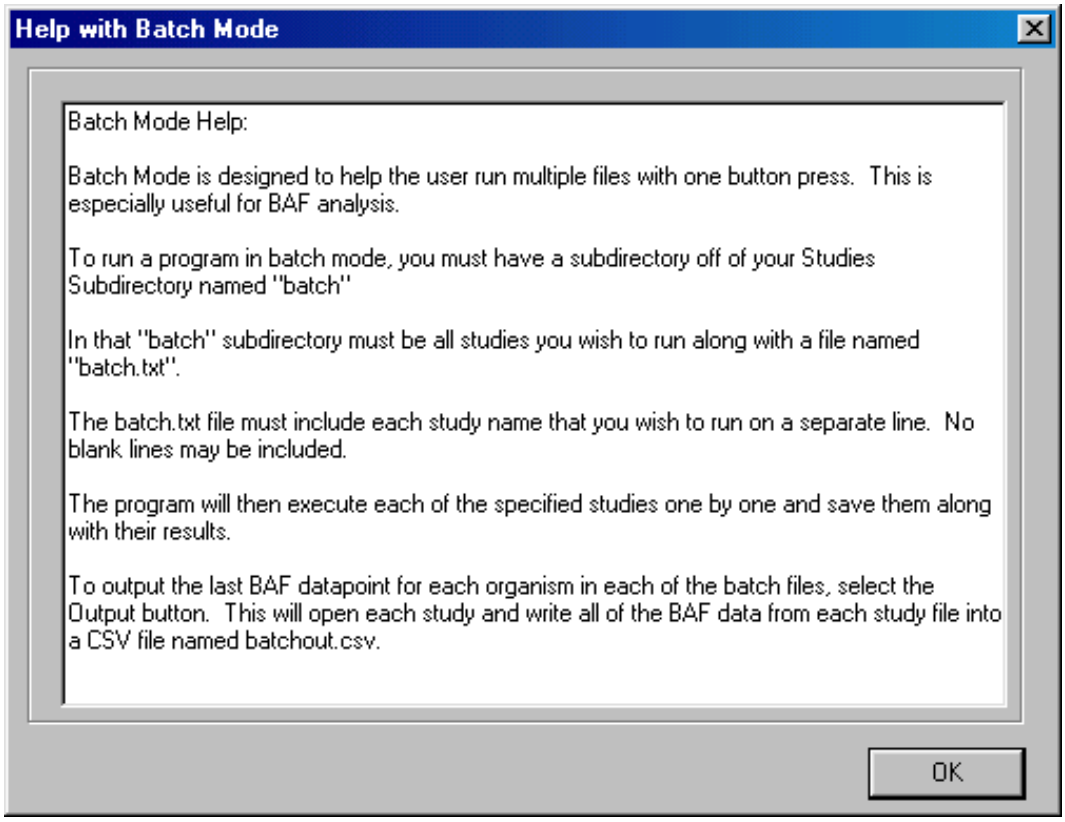


1.7 Running Batch Mode

There are applications where it is desirable to run a series of studies automatically. This can be done by creating a Batch subdirectory under the Study directory and placing studies with appropriately chosen options in it. The subdirectory should also contain a text file labeled "batch.txt" that lists the names of the studies to be run, one to a line. On the menu bar you should click on **Run Batch** on the pull-down **File** window. That will open a window that allows you to **Run in Batch Mode**. You also can save the BAFs and organic-matter partition coefficients (KOMs) to a comma-separated text file *batchout.csv*. (See **Volume 2: Technical Documentation** for discussion of bioaccumulation of organic toxicants, BAFs and KOMs.) The **Help** button will give you context-sensitive help.


AQUATOX v1.02
File Library Help
New
Open...
Close
Save
Save As...
Export
Export Control Results
Print...
Print Setup...
Run Batch
Exit
INFLOW
P
N
OUTFLOW


Run in Batch Mode
Run In Batch Mode
Output KOMs from Batch Mode
Cancel
Help



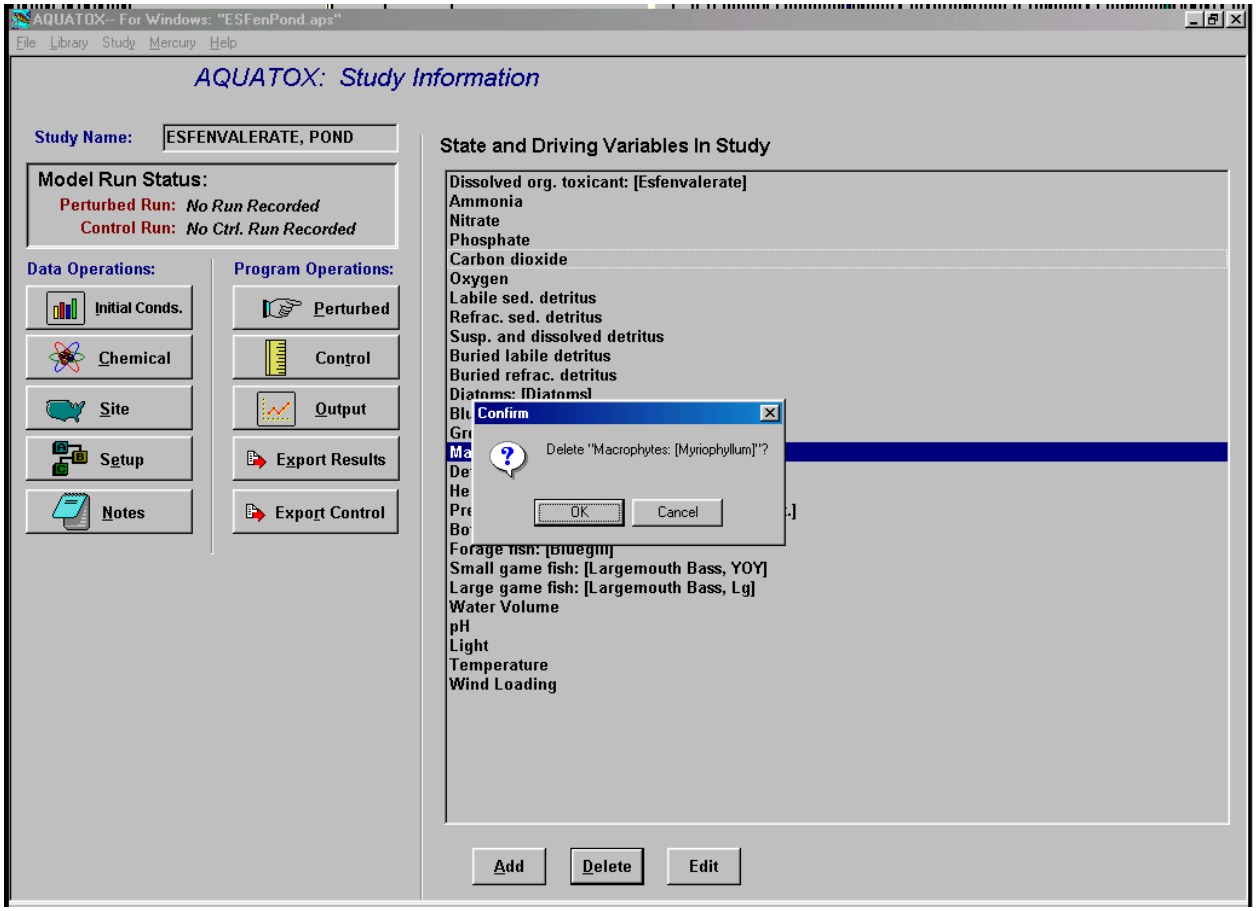
At this point you may experiment with the various buttons and screens. You cannot hurt anything; just don't save the edited data or the study when you exit the screens and AQUATOX unless you **Save As** a different name. On the other hand, if you are more comfortable following directions, read on, doing the operations as you go.

2. MODEL COMPONENTS

2.1 State Variables

Selection—State variables are those ecosystem components that are being simulated. These include organism and detrital compartments and their associated toxicants (which are not listed in the **Study Information** window), nutrients, dissolved oxygen, and other variables traditionally considered driving variables, such as water inflow, temperature, pH, light, and wind.

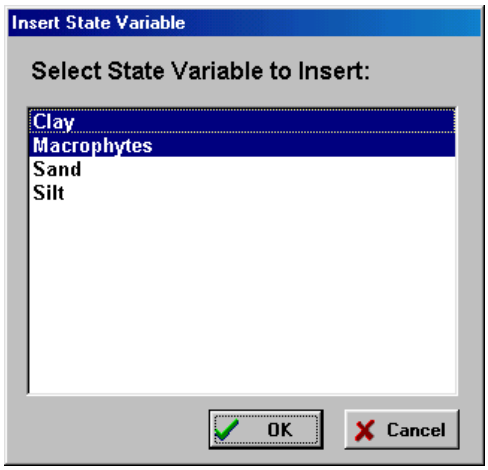
AQUATOX is very powerful because you can add or delete state variables. It is even possible to remove all biotic components in order to model a tank or other sterile system. In general, the fewer state variables, the better. In particular, unnecessary state variables slow down the simulation and create additional requirements for verification. This is especially true for streams, which tend to be more dynamic and therefore slower to simulate. Nevertheless, often it is desirable to model a food web rather than a food chain, for example to examine the possibility of less tolerant organisms being replaced by more tolerant organisms as environmental perturbations occur. The choice of which state variables to model depends to a large extent on the purpose of the modeling application.



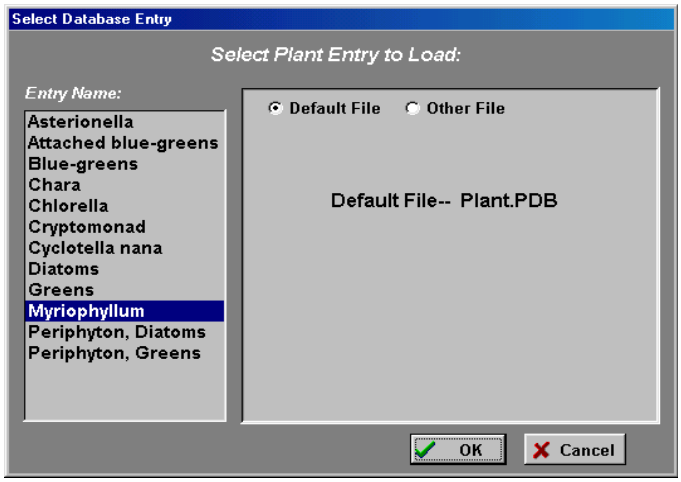
Open the file Esfenpond.aps, if it is not already open. We will remove the macrophyte compartment by highlighting it in the list, clicking on the **Delete** button, and confirming the deletion.

When the change is made, you will see a warning that the **Control Run** is not current. The control run provides a basis of comparison so that the effects of the perturbation can be determined.

Likewise, state variables can be added by clicking on the **Add** button and choosing from the list. Let's add macrophytes back to the list of state variables.

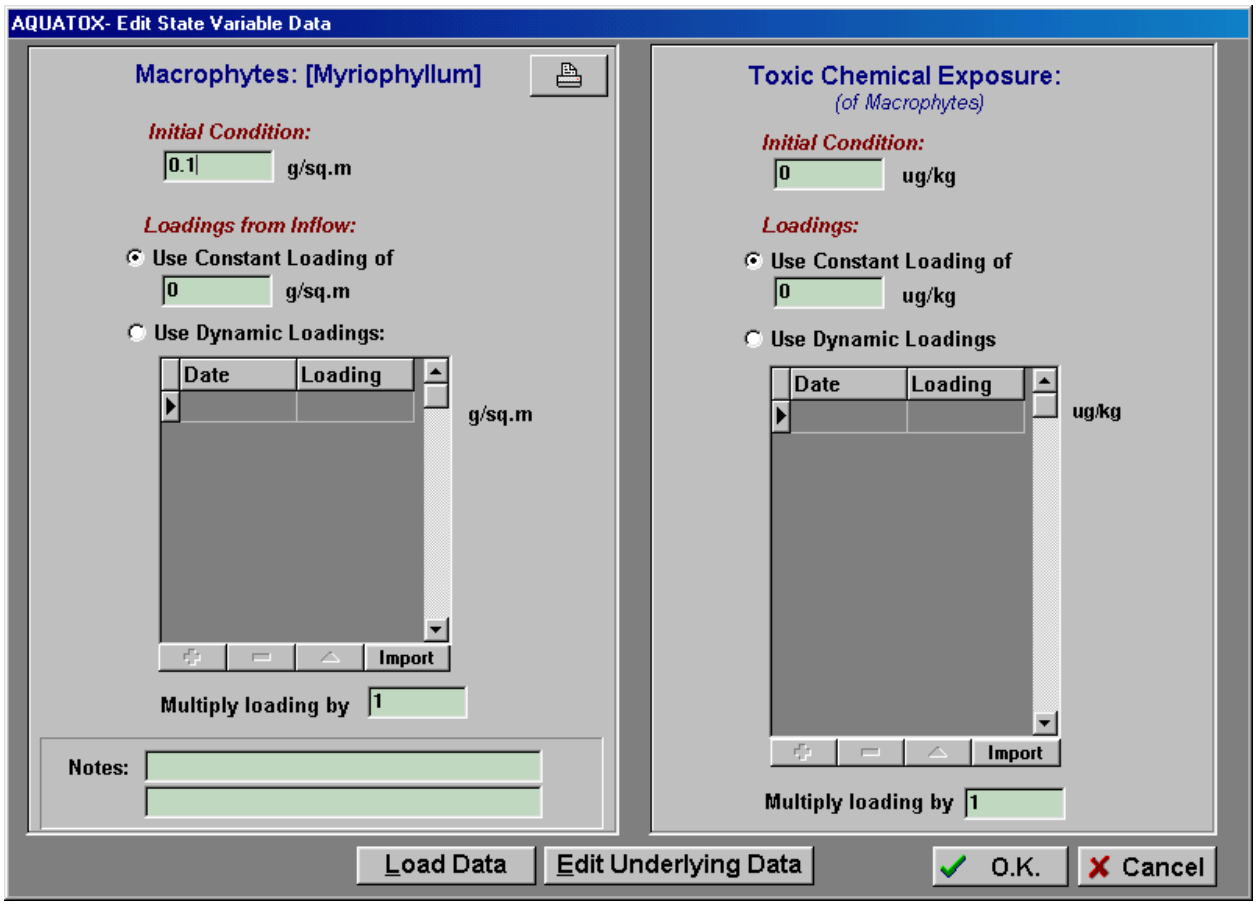


Note that the names of the taxonomic groups and ecologic guilds on the main study screen are followed by the names of the specific groups in brackets. We have to specify the type of macrophyte by highlighting **Macrophytes** and clicking on **Edit**, or by double-clicking on **Macrophytes**. That will give us a double screen representing both the macrophytes and the associated toxicant. Click on **Load Data** to load a specific plant record for macrophytes. In this example, *Chara* and *Myriophyllum* are the only macrophytes listed; we highlight *Myriophyllum* and click on **OK**. If there is no selection made you will receive an error message indicating that there is no data associated with the state variable **Macrophyte.**

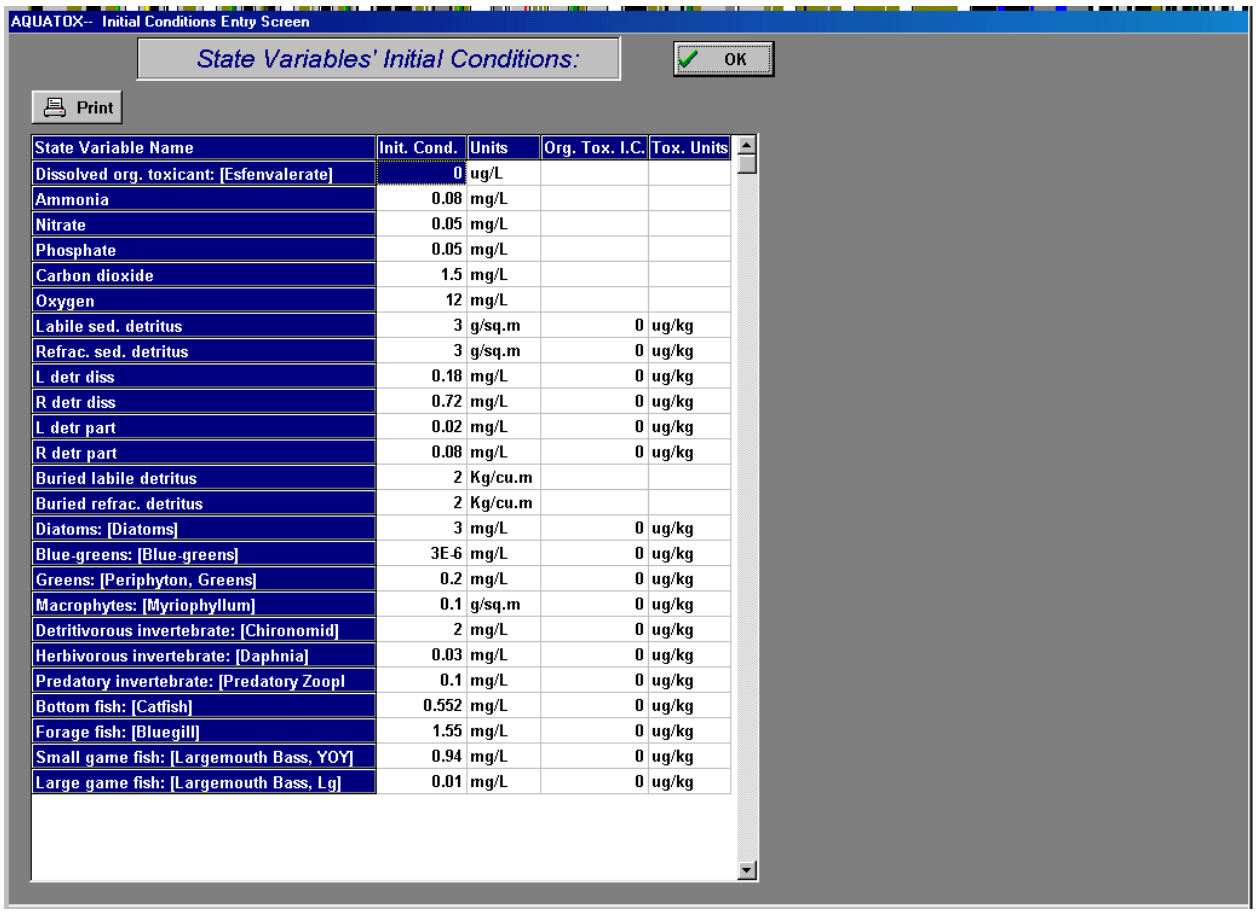


Initial Conditions—To continue with our macrophyte example, we should enter a value for the biomass of macrophytes present at the beginning of the simulation; if the value is left as 0 and there is no loading, then macrophytes would not be simulated. The initial condition will depend on when the simulation starts (which is specified in **Setup**). In this example we will enter a value of 0.1 g/m^2,

which is appropriate for *Myriophyllum* in a temperate pond at the beginning of the growing season.



The **Initial Conditions** screen provides a useful way of displaying all state variables. In order to avoid conflicts with other windows, you cannot edit the initial conditions in this screen; that is reserved for the loading screens.

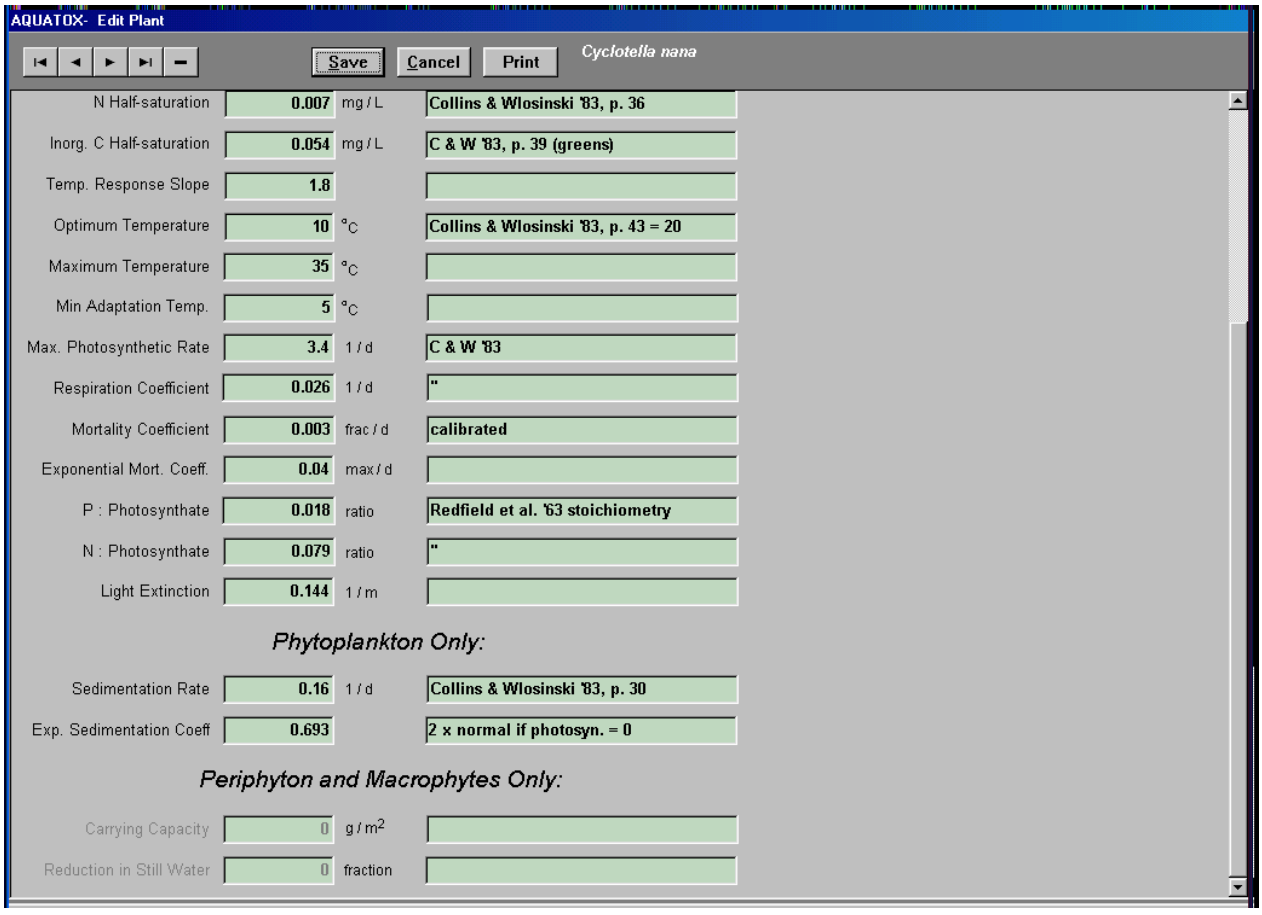


State Variable Name	Init. Cond.	Units	Org. Tox. I.C.	Tox. Units
Dissolved org. toxicant: [Esfenvalerate]	0	ug/L		
Ammonia	0.08	mg/L		
Nitrate	0.05	mg/L		
Phosphate	0.05	mg/L		
Carbon dioxide	1.5	mg/L		
Oxygen	12	mg/L		
Labile sed. detritus	3	g/sq.m	0	ug/kg
Refrac. sed. detritus	3	g/sq.m	0	ug/kg
L detr diss	0.18	mg/L	0	ug/kg
R detr diss	0.72	mg/L	0	ug/kg
L detr part	0.02	mg/L	0	ug/kg
R detr part	0.08	mg/L	0	ug/kg
Buried labile detritus	2	Kg/cu.m		
Buried refrac. detritus	2	Kg/cu.m		
Diatoms: [Diatoms]	3	mg/L	0	ug/kg
Blue-greens: [Blue-greens]	3E-6	mg/L	0	ug/kg
Greens: [Periphyton, Greens]	0.2	mg/L	0	ug/kg
Macrophytes: [Myriophyllum]	0.1	g/sq.m	0	ug/kg
Detritivorous invertebrate: [Chironomid]	2	mg/L	0	ug/kg
Herbivorous invertebrate: [Daphnia]	0.03	mg/L	0	ug/kg
Predatory invertebrate: [Predatory Zoopl	0.1	mg/L	0	ug/kg
Bottom fish: [Catfish]	0.552	mg/L	0	ug/kg
Forage fish: [Bluegill]	1.55	mg/L	0	ug/kg
Small game fish: [Largemouth Bass, YOY]	0.94	mg/L	0	ug/kg
Large game fish: [Largemouth Bass, Lg]	0.01	mg/L	0	ug/kg

Parameters—These provide values for coefficients in the process equations. Although default values are given, the user has great flexibility in specifying values to represent site-specific species or groups. We already have seen the screen for chemical parameters as an example of using the Library. Instead of loading the general library record, we could have loaded the study-specific record by clicking on **Chemical** or by double-clicking on **Dissolved org. toxicant** in the state variable list and then choosing **Edit underlying data**. In the following examples we will examine a record from each of the other libraries. A record can be down-loaded into a study from a library by choosing **Load data** on the Edit State Variable Data screen.

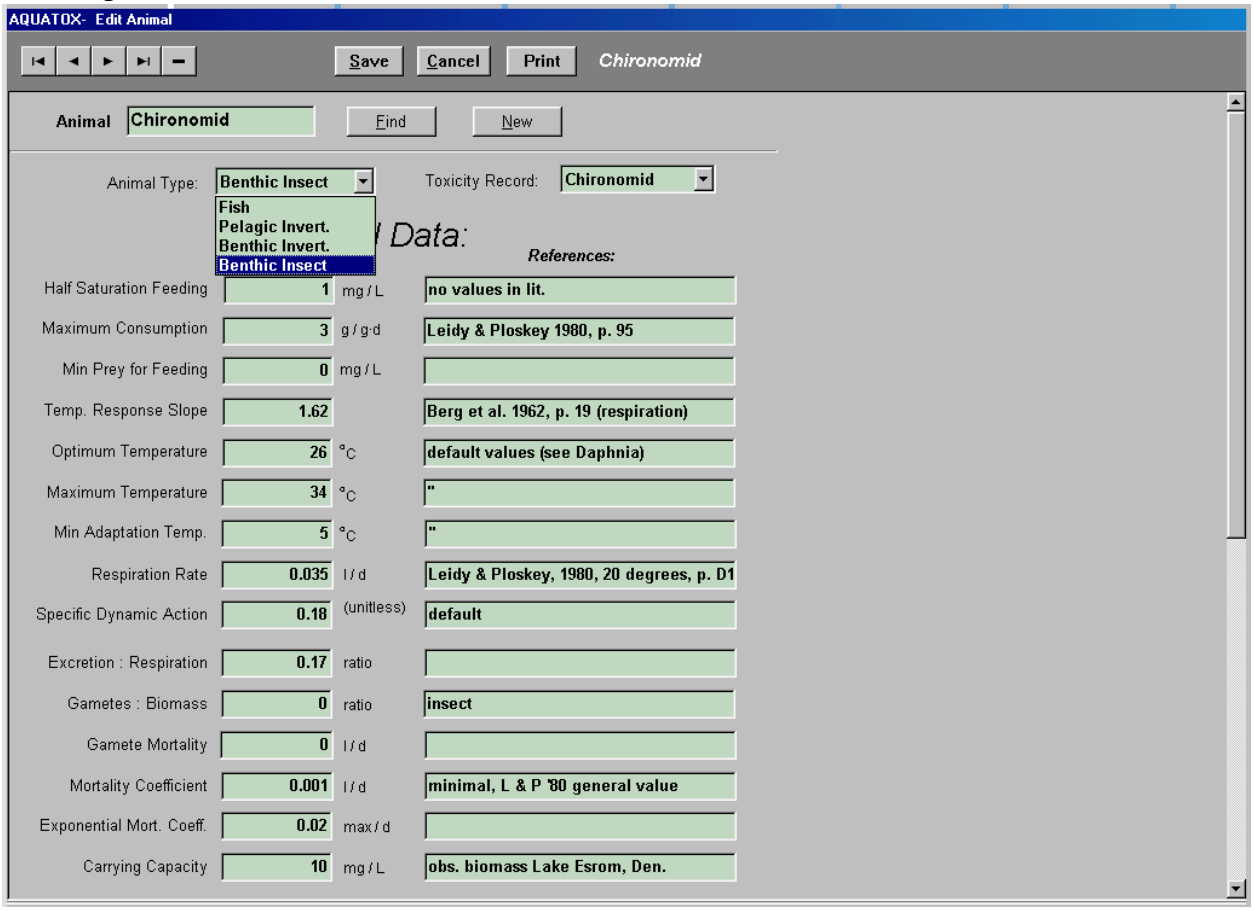
We will examine first the parameter screen for plants. Choose **Plants** from the **Library** menu, then move to *Cyclotella nana* (this is a common diatom, but we could just as easily have chosen Diatom and gotten more general parameter values). Two fields near the top of the screen require explanation. If you click on the arrow to the right of **Plant type**, you will be given a choice. The choice of **Plant type** is important because different types have different physical or biological processes that apply to them. For instance, phytoplankton are subject to sinking, but not periphyton, which are attached to a surface. Conversely periphyton are limited somewhat by very slow current velocity; but not phytoplankton, which are adapted to still water.

Less obvious is the **Toxicity Record**; again, clicking on the arrow to the right of the field will give you several choices. The intent is to associate the organism record with one of the limited number of organisms for which there might be toxicity data or procedures for estimating toxicity. In this instance, if you choose **Diatoms** the model will utilize the toxicity data (e.g., EC50) for Esfenvalerate to Diatoms, as listed on the **Toxicity Record** portion of the **Chemical Properties** screen.

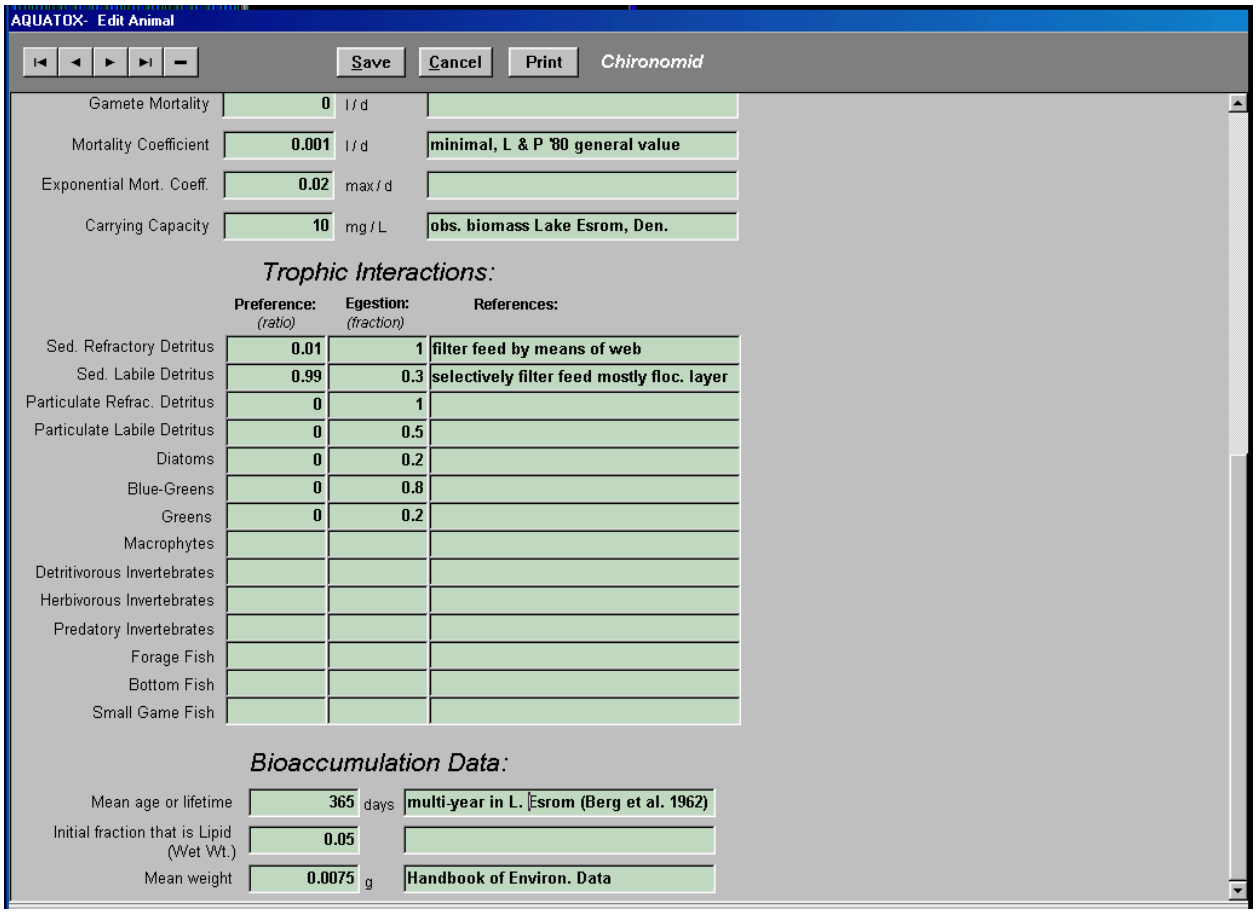


The given parameter values are provided to get you started; if you have more appropriate values, you should use them! Those parameters that do not pertain to phytoplankton are dimmed. If you try to enter a value for **Reduction in still water**, for example, you will find that the field cannot be edited.

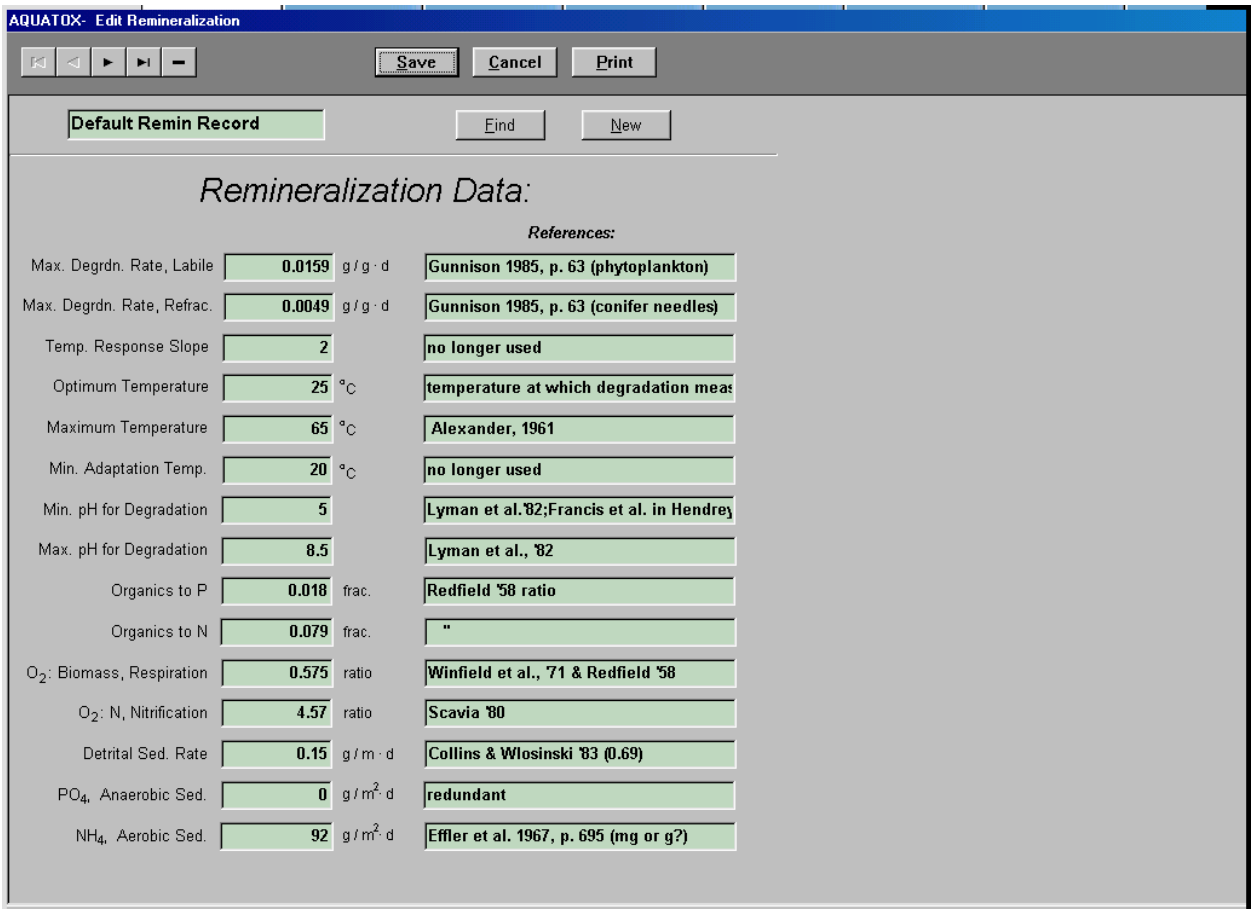
Next we will locate the record for Chironomid from the Animal Library. Click on **Animal Type** to see the pull-down menu. Chironomids have aquatic larvae, so **Benthic insects** is chosen; this is important because emergence is simulated by AQUATOX for insects as a loss term, but does not apply to other animals. Note that the drop-down menu for **Toxicity Record** here includes an **Other** selection. If there is no clear association and you have toxicity data, you should choose **Other** and enter the data under **Other** in the **Toxicity** part of the **Chemical** screen. Click on the scroll bar to the right to see the rest of the Plant screen.



Scroll down to see the rest of the screen. The trophic interaction table is important because it defines the food-web relationships and assimilation efficiencies. Freshly sedimented phytoplankton are an important food source for chironomids; these are modeled as labile sediment organic matter in AQUATOX. The **Bioaccumulation Data** section contains parameters relevant to bioaccumulation of organic toxicants, only one of which (**Initial fraction that is Lipid)** is sensitive. The model is not sensitive to the longevity of the insects because emergence is a function of growth rate, which depends on local, seasonally varying conditions. Likewise, mean weight can only be approximate across all instars because it will vary greatly during the growing season.



Finally, we will examine the default remineralization screen. Because the parameters are global there is little need to change them for a site, unless the organic material is quite different or there is some reason that the microflora might have adapted to abnormal conditions, such as a thermal spring or acid mine drainage.

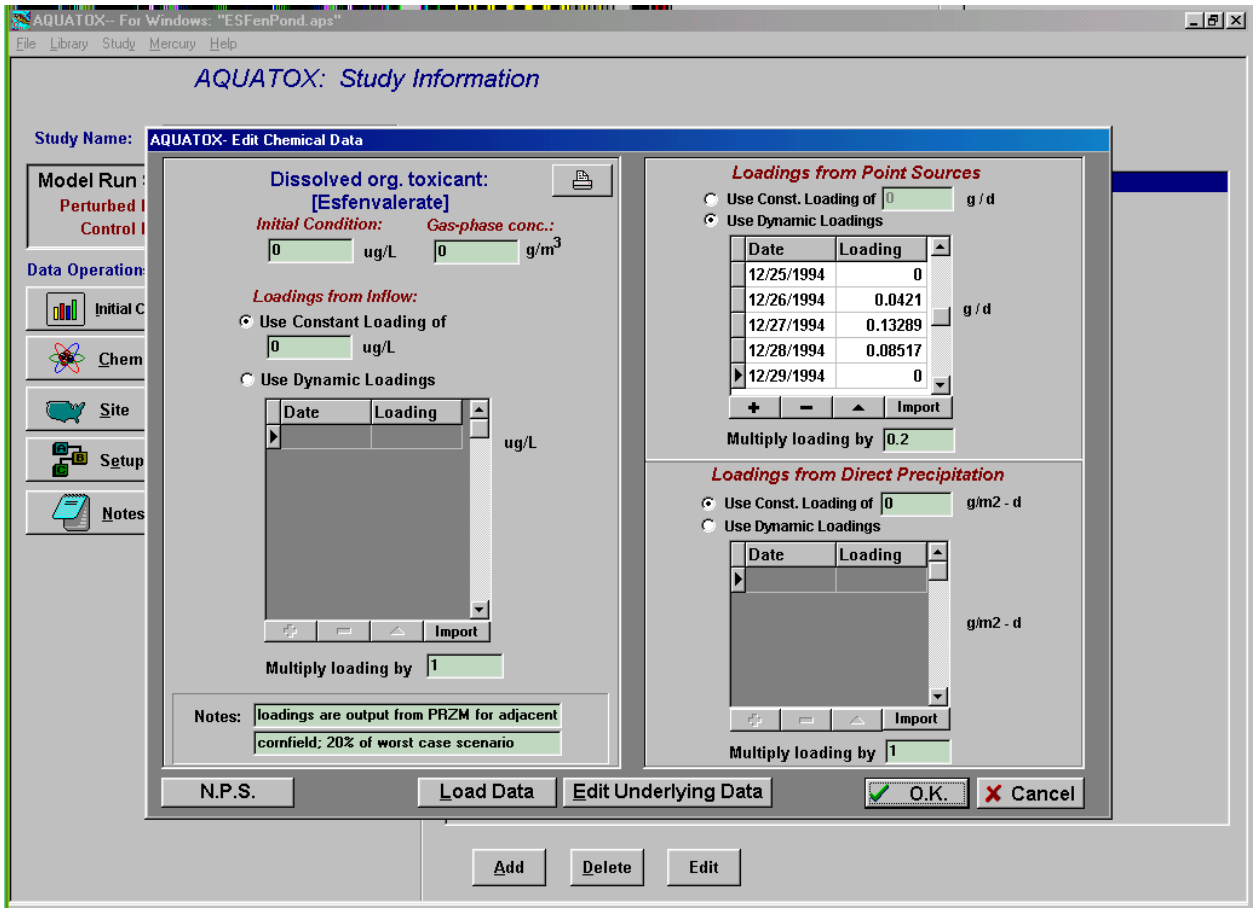


Loadings— Double-click on **Dissolved org. toxicant** or on the **Chemical** button on the main screen to bring up the **Edit Chemical Data** screen, and to examine the various options for loadings to the system. Pollutant loadings can be entered as constant or dynamic loadings in several different forms. The pollutant can be entered as a concentration in the dissolved phase (or loosely bound to suspended sediment); the water inflow and the site volume are then used by the model to compute the loading per unit volume. The gas-phase concentration is used to compute atmospheric exchange; ordinarily concentration in the atmosphere can be considered to be 0, although some pollutants such as PCBs may have significant atmospheric concentrations.

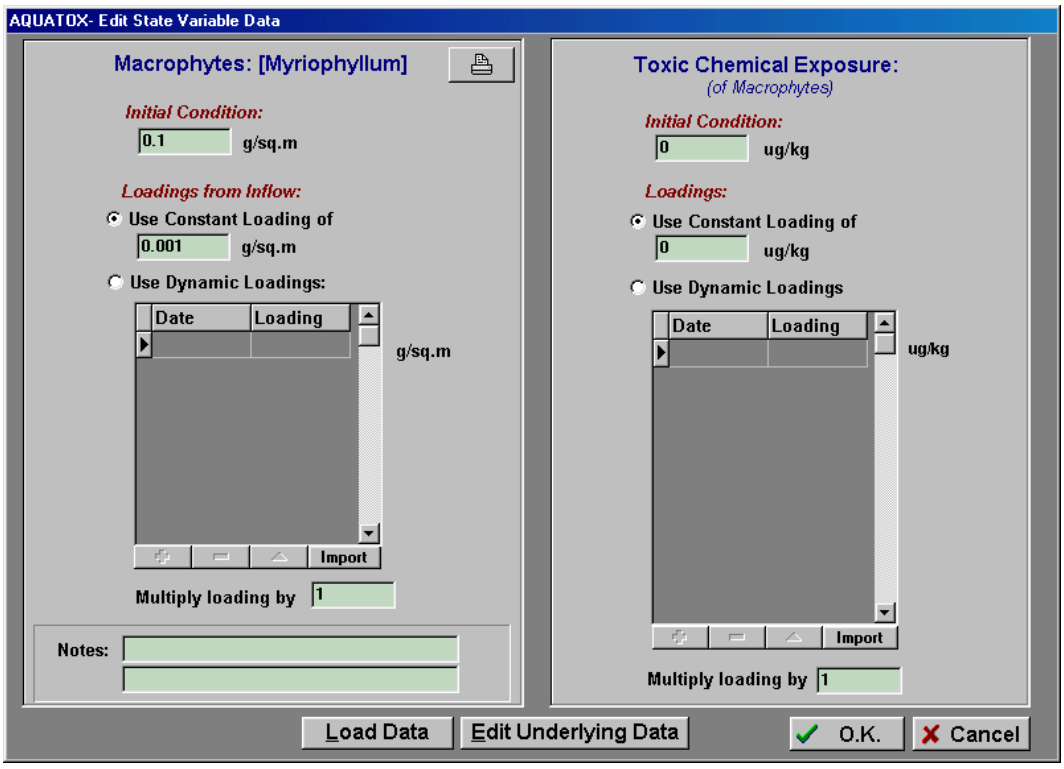
Point-source loadings are mass per day (g/d) for the entire site; they are divided by the site volume to obtain the loading per unit volume. In this example, dynamic loadings from a point discharge as calculated by the PRZM model are entered. Note that the dynamic loadings are interpolated, so if the intent is to represent a spike such as from storm runoff on a particular day, then the loading should be bracketed by "0" loadings. The model assumes that the loadings "wrap around" with an annual cycle and that the last loading can be interpolated to the first loading as if it were in the succeeding year. Exercise caution when modeling multiple years, but you only have loadings data from one or a few years. Sporadic loadings, which would only be expected in that one particular year, may inappropriately be repeated in successive years. If you do not wish loadings to be repeated, enter values ("0" or otherwise) for the first and last days of the simulation. The dynamic loadings in this example were entered by hand; an excellent alternative is to download or prepare

a file external to the model and import it into the study using the **Import** button. This procedure is described in detail later.

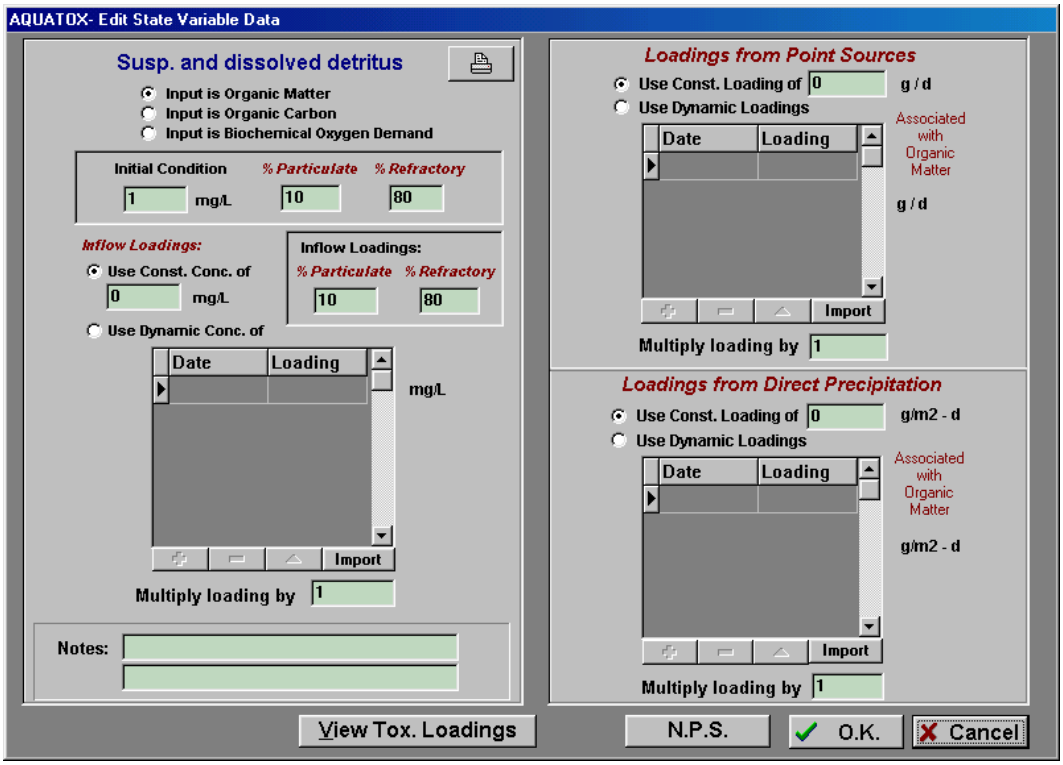
Another potential pollution loading source is from direct precipitation. These are given as g/m^2 d because AQUATOX does not explicitly consider precipitation. Click on **N.P.S.** to toggle to the non-point source screen, which is in g/d.



Let's go back to the Macrophyte Edit State Variable screen. Ordinarily we think of loadings as pertaining only to chemicals and freely moving organisms such as plankton and fish. However, it is often desirable to enter a small constant loading to serve as a "seed" if the population or group is killed off entirely by a toxicant or adverse environmental conditions. This is especially important for macrophytes that suffer winter die-back. Therefore, we will use a value of 0.001 g/m^2 as a constant loading. This is small enough that it will not affect the results during the growing season, but it is large enough to represent regeneration from rhizomes, which are not modeled explicitly.

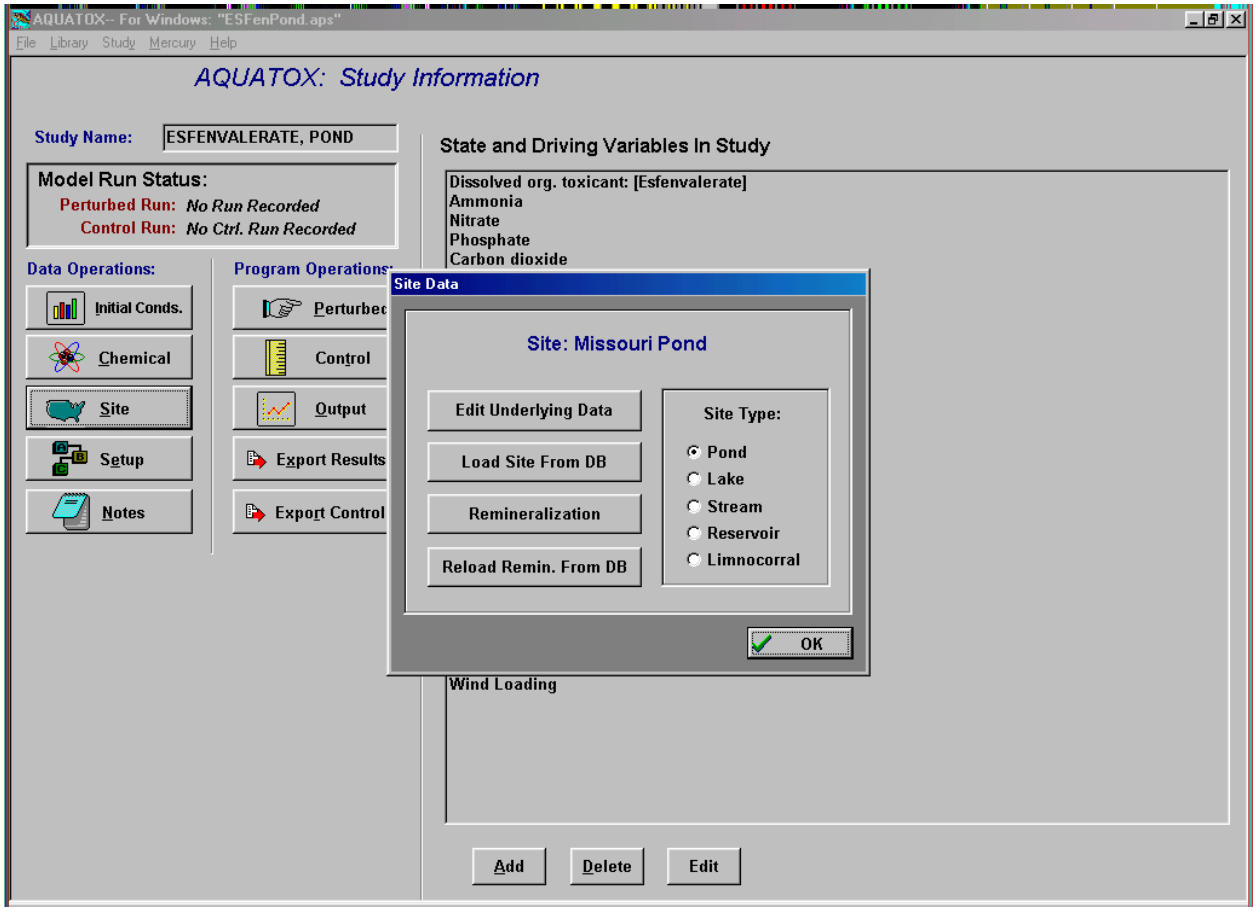

AQUATOX- Edit State Variable Data
Macrophytes: [Myriophyllum]
Initial Condition:
0.1
g/sq.m
Loadings from Inflow:
Use Constant Loading of
0.001
g/sq.m
Use Dynamic Loadings:
Date
Loading
g/sq.m
Import
Multiply loading by
1
Notes:
Toxic Chemical Exposure:
(of Macrophytes)
Initial Condition:
0
ug/kg
Loadings:
Use Constant Loading of
0
ug/kg
Use Dynamic Loadings
Date
Loading
ug/kg
Import
Multiply loading by
1
Load Data
Edit Underlying Data
O.K.
Cancel

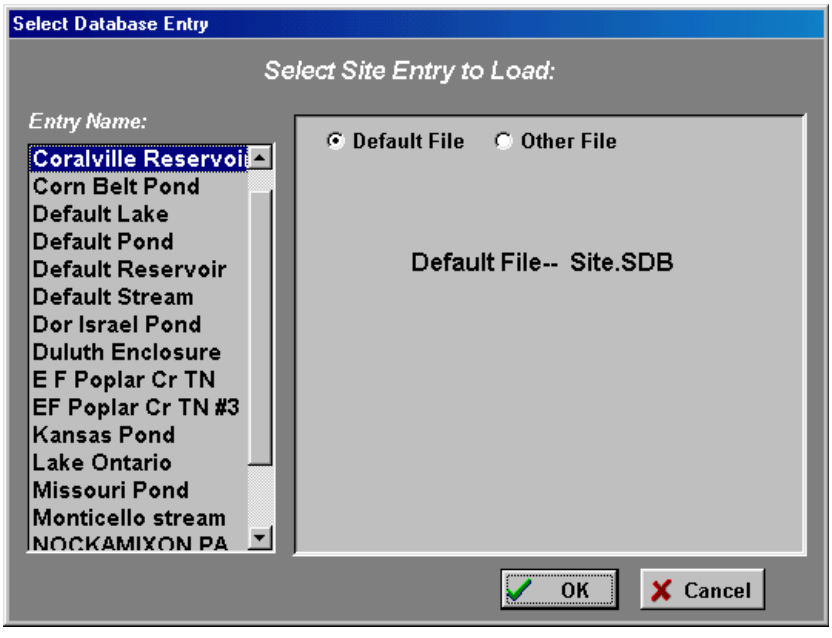
Perhaps the most confusing, yet flexible, loading screens are those for suspended and dissolved detritus. In an effort to minimize data requirements, the screens combine several compartments: suspended and dissolved refractory and labile detritus, defined as percentages. AQUATOX will make the appropriate conversions from BOD, organic carbon, and organic material, and partition them among refractory and labile particulate and dissolved fractions to provide input to the model run.



2.2 Sites

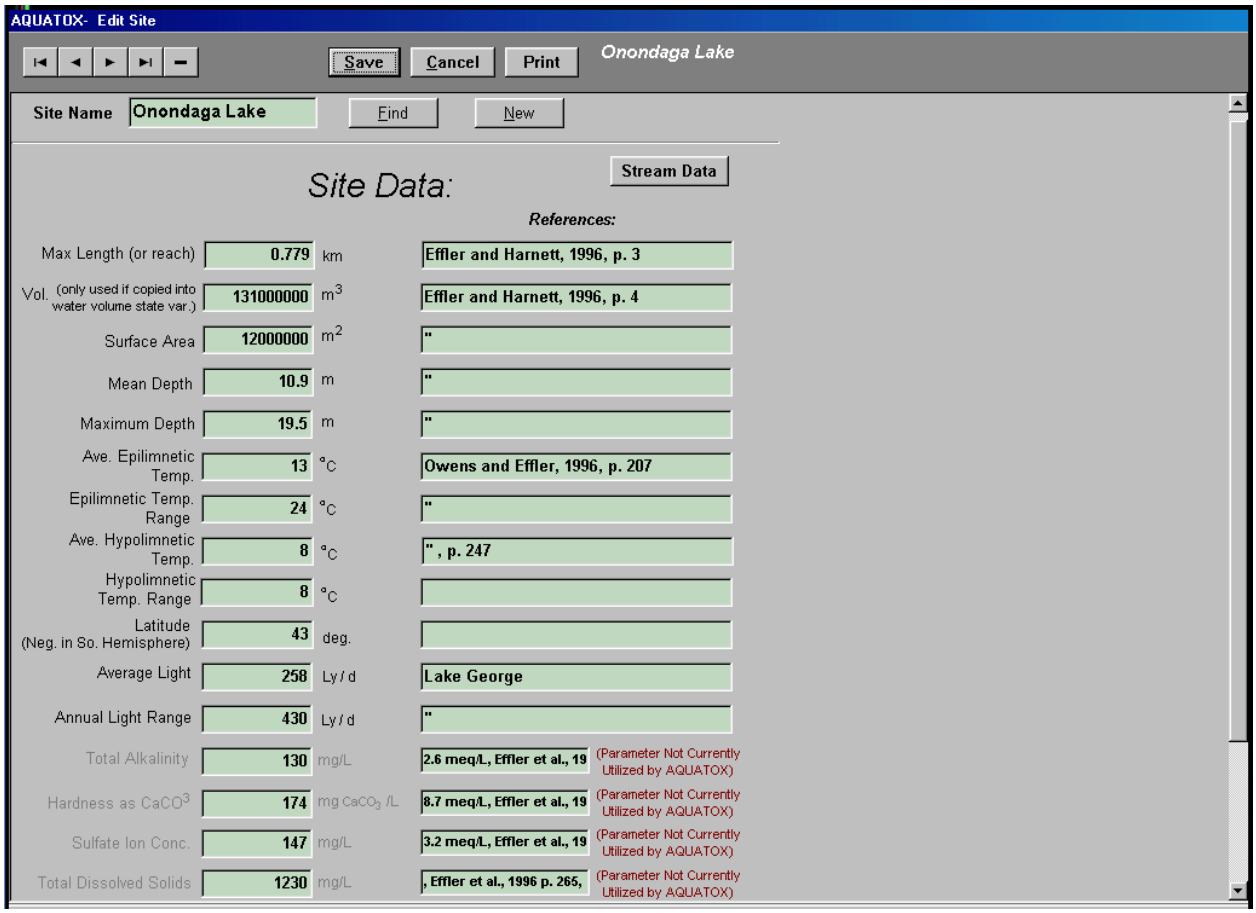
Selection—Several default sites are provided as part of the AQUATOX database. These can be edited and additional ones can be created in **Library** mode. They can be loaded into a **Study** by clicking on the **Site** button. The **Site Type** is used at this time to indicate a baseline extinction coefficient for the water and, for streams, to enable computation of discharge-related characteristics; it does *not* serve as a filter for the site choices that are presented when one chooses **Load Site from DB**.


AQUATOX-- For Windows: "ESFenPond.aps"
File Library Study Mercury Help
AQUATOX: Study Information
Study Name: ESFENVALERATE, POND
Model Run Status:
Perturbed Run: No Run Recorded
Control Run: No Ctrl. Run Recorded
State and Driving Variables In Study
Dissolved org. toxicant: [Esfenvalerate]
Ammonia
Nitrate
Phosphate
Carbon dioxide
Data Operations:
Initial Conds.
Chemical
Site
Setup
Notes
Program Operations:
Perturbec
Control
Output
Export Results
Export Control
Site Data
Site: Missouri Pond
Edit Underlying Data
Load Site From DB
Remineralization
Reload Remin. From DB
Site Type:
Pond
Lake
Stream
Reservoir
Limnocorral
OK
Wind Loading
Add
Delete
Edit


Select Database Entry
Select Site Entry to Load:
Entry Name:
Coralville Reservoi
Corn Belt Pond
Default Lake
Default Pond
Default Reservoir
Default Stream
Dor Israel Pond
Duluth Enclosure
E F Poplar Cr TN
EF Poplar Cr TN #3
Kansas Pond
Lake Ontario
Missouri Pond
Monticello stream
NOCKAMIXON PA
Default File
Other File
Default File-- Site.SDB
OK
Cancel

Site Characteristics—Each site can be characterized by a small number of site constants. These can be seen and edited by clicking on **Edit Underlying Data** in the **Site Data** window, or they can be loaded from the **Library**. There is some redundancy in that **Volume**, **Area**, and **Mean Depth** all have to be specified. Based on mean and maximum depth, the bathymetry of the site is computed. Volume is a state variable and can be computed in a variety of ways (accessible through the volume loading screen); however, one option is to set it to a constant using the value provided in the site screen (see **2.3 Driving Variables**).

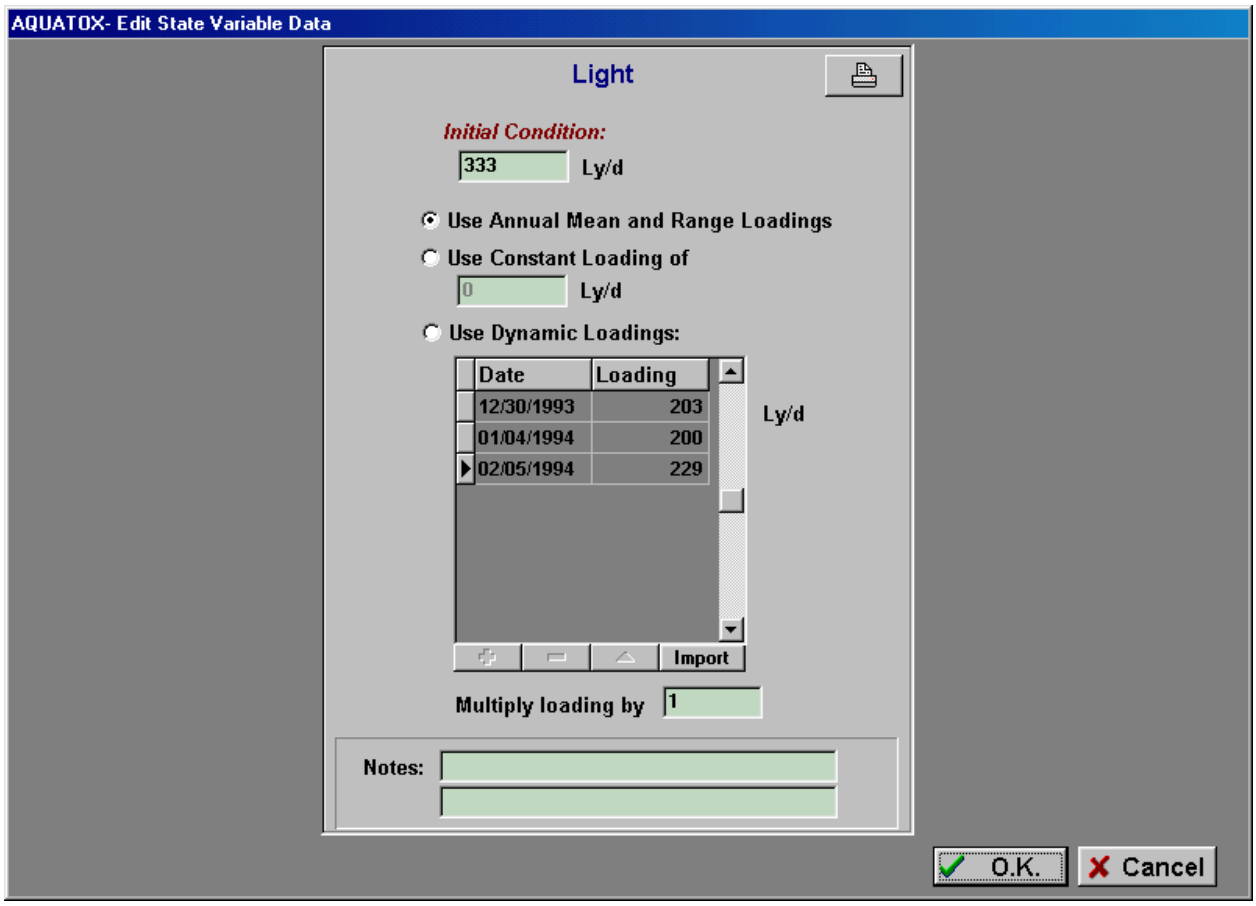
Both epilimnetic and hypolimnetic temperature parameters have to be specified, even for streams and ponds, where they can be set equal. Given observed annual means and ranges for temperature and light, seasonal fluctuations are computed. These are not computed from the latitude because of local and regional differences in elevation, cloud cover, and maritime or continental climatic conditions. **Latitude** is used to compute the seasonal variation in day length. The **Max. Length** is the distance, usually the long axis, across which wave buildup can occur; it determines the depth of mixing in stratified systems. Some variables are not used at this time and are so indicated.



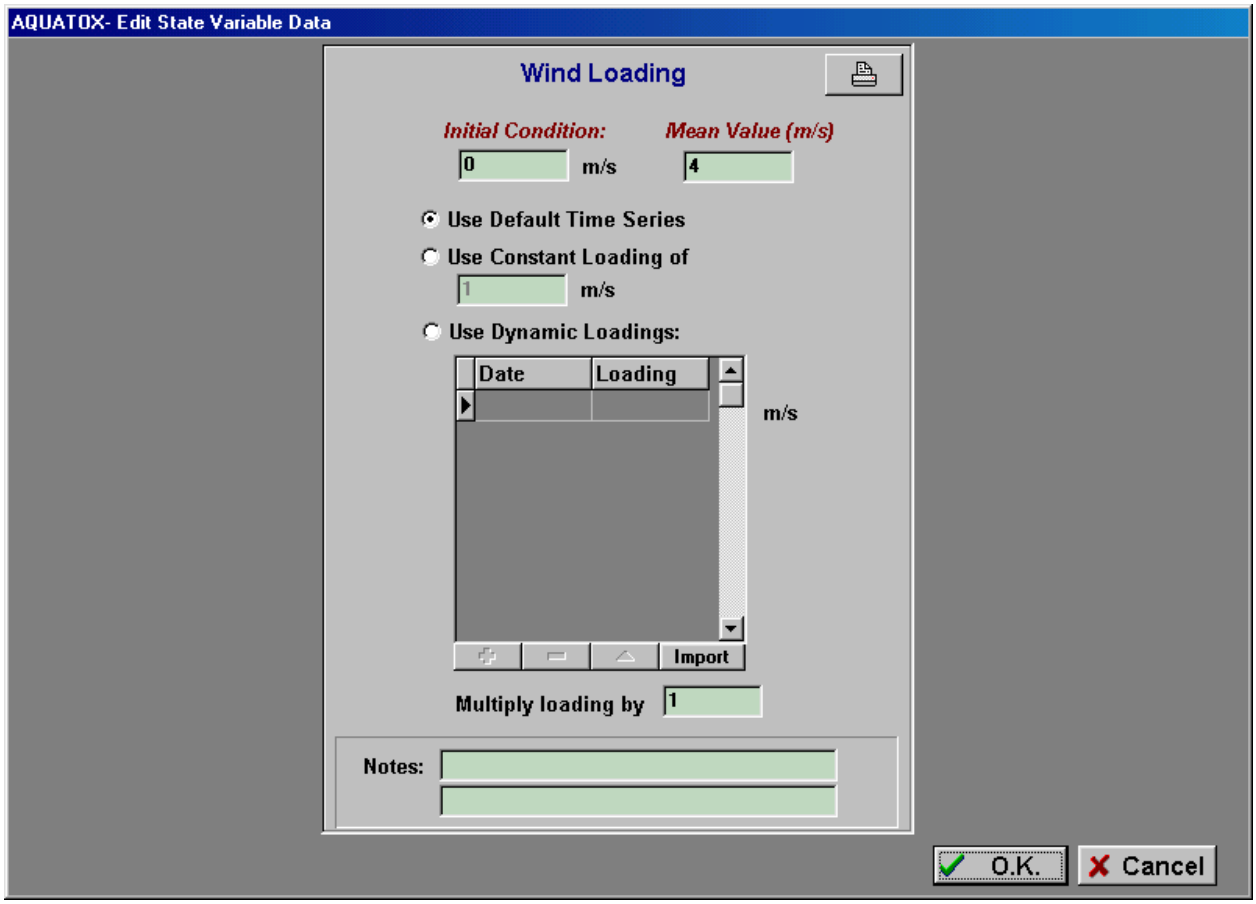
If modeling a stream, information on the type of channel and slope can be supplied by clicking on the **Stream data** button.

2.3 Driving Variables

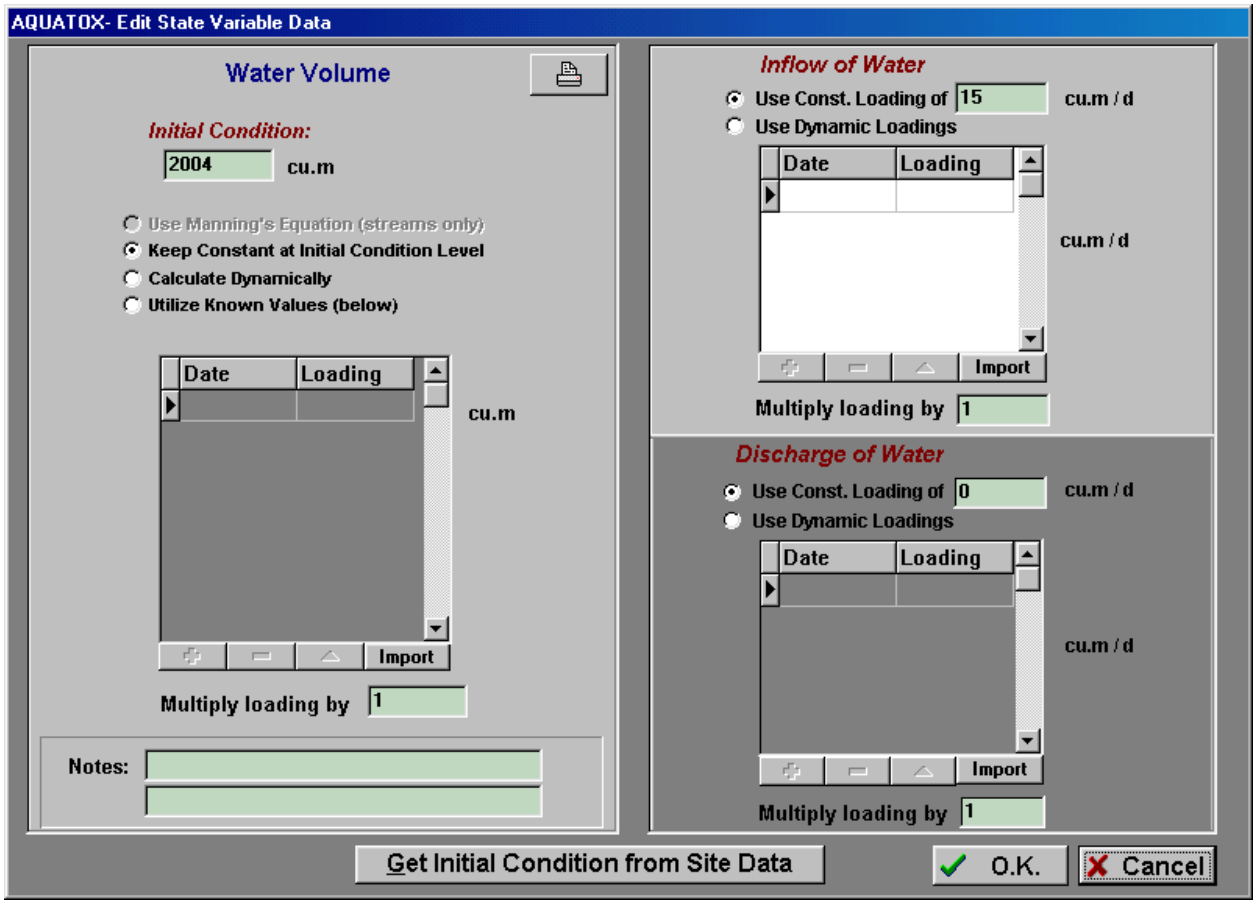
The traditional driving variables (light, water temperature, wind, pH, and water volume) are listed with the state variables on the **Study Information** (main) screen. This was done because it simplified the data structure, and it provides for expansion of the model to compute these variables using differential equations. As mentioned above, light and temperature are computed from annual means and ranges using simple sinusoidal functions. They also can be specified by the user as constant or variable loadings. The **Edit** window is called by double-clicking on the appropriate item in the list.



As a default, wind is computed using a complex Fourier series of sines and cosines for a 140-day repeating period with a user-supplied mean value. Dynamic loadings of observed values can be entered or imported. At this time pH is a site constant or loading.

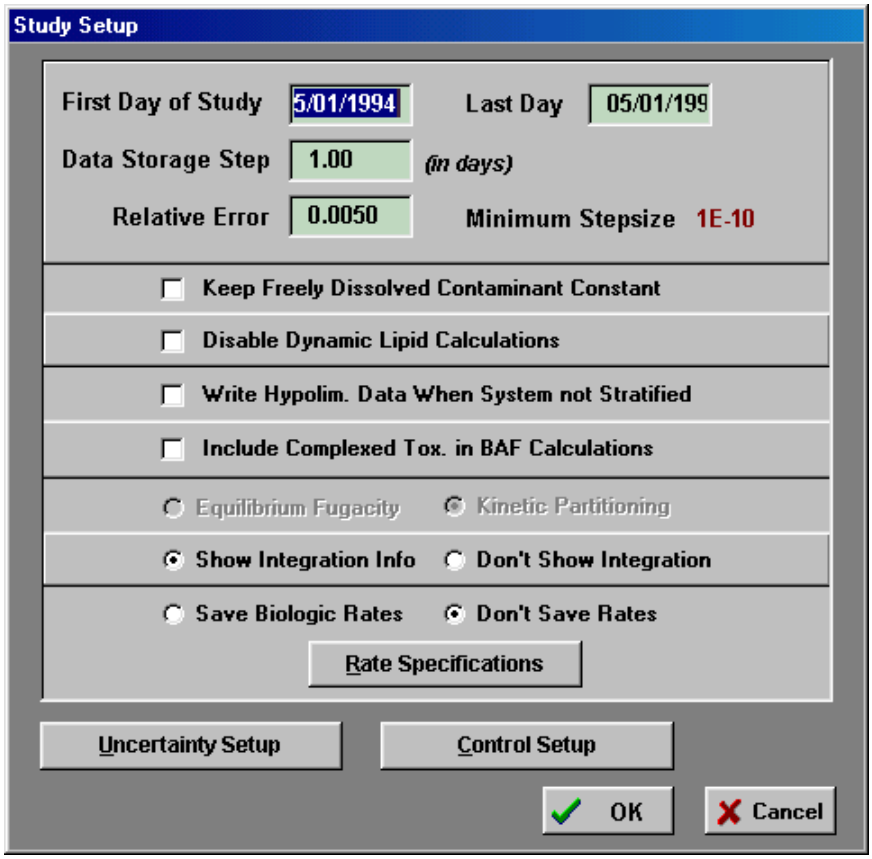


Inflow, outflow, and changes in volume can be represented by a variety of options. In this simple example, the volume is kept constant. Although inflow is provided as a constant, it can be overridden by the model if there is insufficient inflow to offset evaporation (an annual site constant set by the user). Likewise, discharge is computed to maintain the volume with high inflow. An example of dynamically specified volume will be given later.



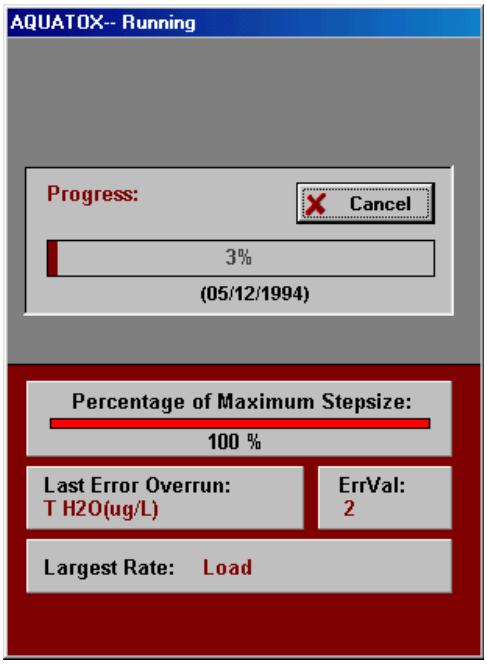
2.4 Setup

Before you execute the model, you should check various settings by clicking on **Setup**. At the top of the setup screen you can modify the first and last days of the simulation. Use a 4-digit year designation to avoid any confusion between the years 1900 and 2000; the model will interpret "/00" as "/2000." The Data Storage Step defines how often the results are saved; it is usually one day, but can be varied to save space or show high frequency results. AQUATOX interpolates variable-step output to obtain the desired interval. The Relative Error is the acceptable error in the simulation; if it is not achieved in a particular time step, the variable Runge-Kutta routine decreases the step size and tries again. If the relative error is too large, the results may be erroneous; if it is too small, the run time may be too long. Usually a value between 0.005 and 0.0005 is appropriate, but you may wish to experiment for a particular application.

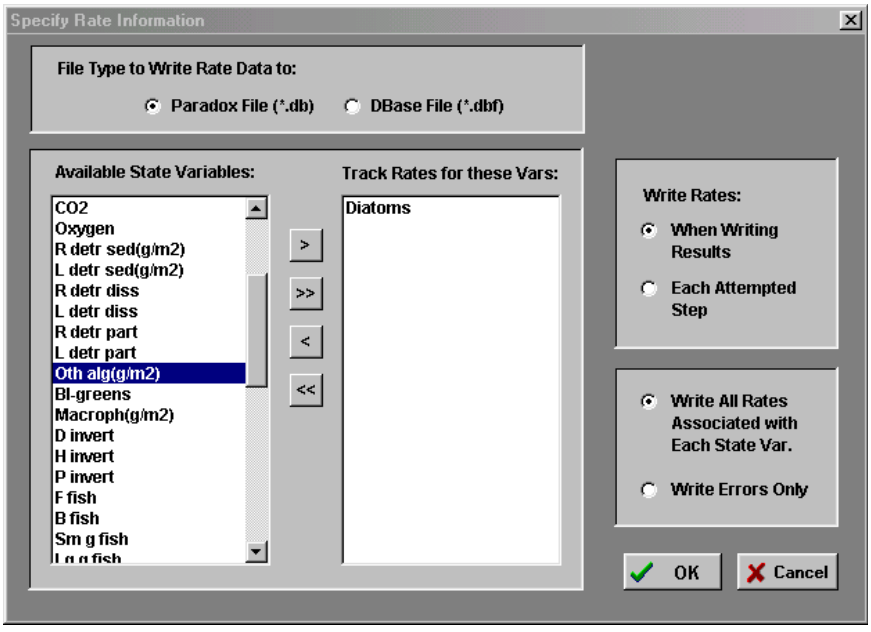


What follows are three choices for computing bioaccumulation factors (BAFs) and a choice for saving output. If you wish to compute steady-state BAFs, you may wish to hold the freely dissolved contaminant constant; this was done in an application concerning PCBs in Lake Ontario (see **Volume 3: Model Validation Reports** document). AQUATOX calculates time-varying lipid fractions in fish, but those calculations can be disabled and default or user-supplied initial values can be used. The older literature often did not distinguish between freely dissolved contaminants and those complexed with dissolved organic matter. You may choose to include the complexed contaminant in computing BAFs so that the results are directly comparable with the older literature values. In plotting output for stratified systems it is usually more pleasing to plot continuous values for the hypolimnion, even when the system is not stratified. This is done by duplicating epilimnion values for the hypolimnion when the system is well mixed; however, that takes additional storage, so you may choose not to duplicate those data points.

Fugacity and kinetic partitioning are grayed out because the model only represents kinetic partitioning now. If you click on **Show Integration Info.** you will be able to see what time steps are used in solving the differential equations and what rates and associated relative errors are causing the integration to slow down while the model is running.



You may save biologic (and chemical) rates for examination with a spreadsheet program. Choose **Save Biologic Rates** and click on **Rate Specifications** to designate those state variables for which you want the additional output. Don't save rates for all state variables or the output will be voluminous! Usually you would save rates for each output step, by choosing **When Writing Results**. However, you can save rates for each step in the solution of the differential equations, that is, **Each Attempted Step**. You also can choose to save just the errors associated with each state variable. These latter choices are useful only if you are concerned with the details of the numerical analysis.

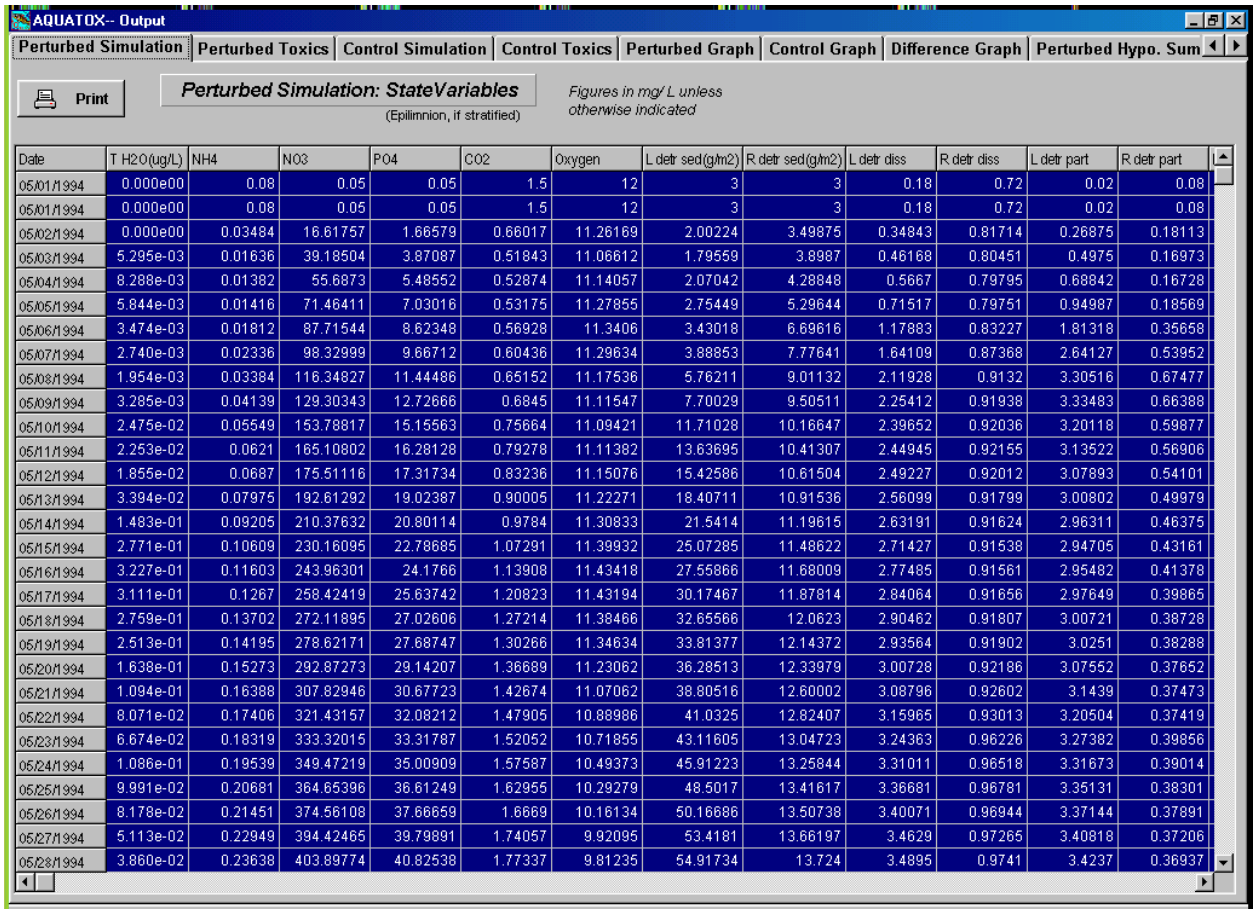


Uncertainty and Control setups are complex and are covered under **Applications**.

2.5 Output

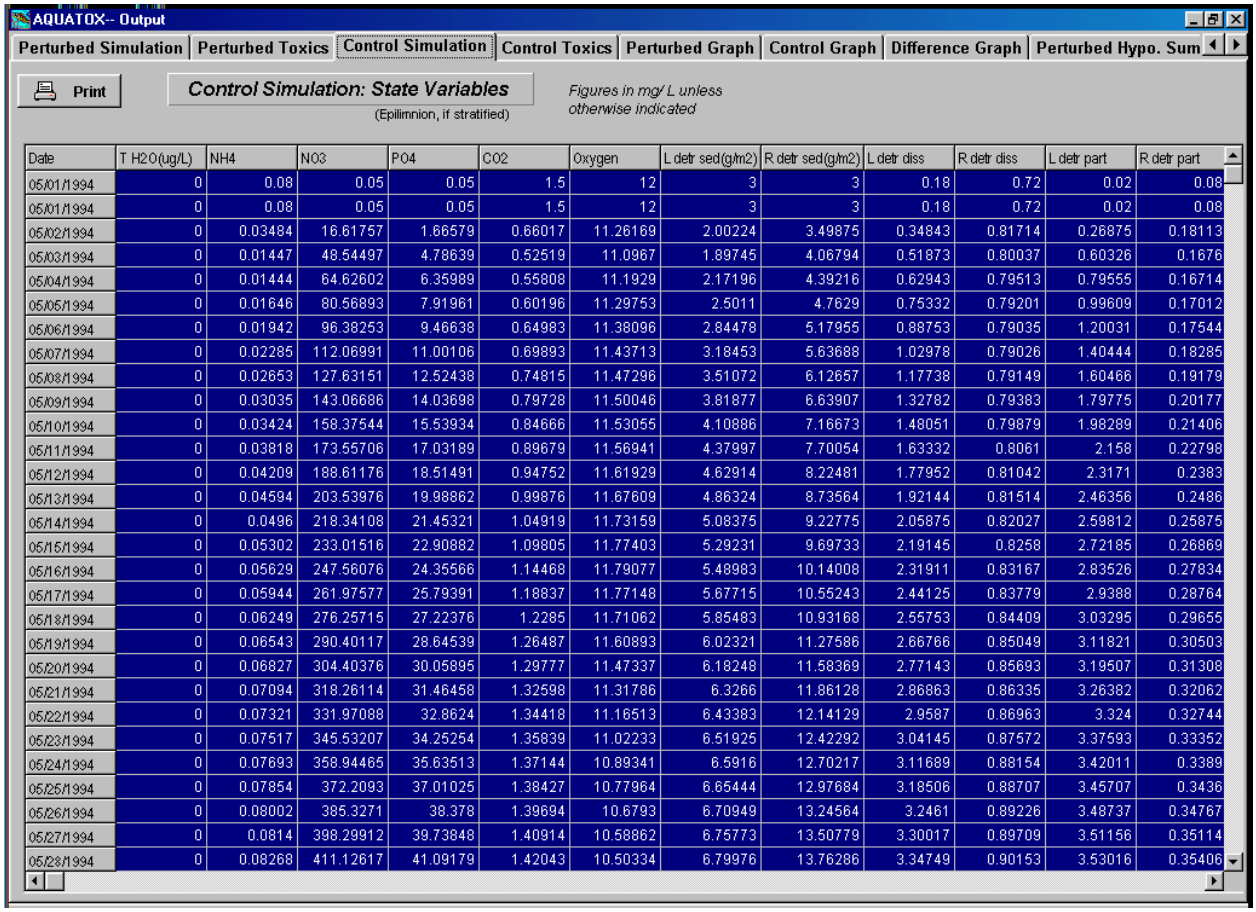
AQUATOX takes advantage of the Borland database engine to provide a rich selection of output screens. Click on **Output** in the main screen to see these. Unfortunately, because of the complexity of the data and the number of output configurations, it may take several minutes to format and load the output on a slower computer.

Tables—First let's examine the **Perturbed Simulation** table. It gives the values for each of the state variables using the reporting step specified in the **Setup** screen; the default step is one day. The first row in the table gives the initial conditions.



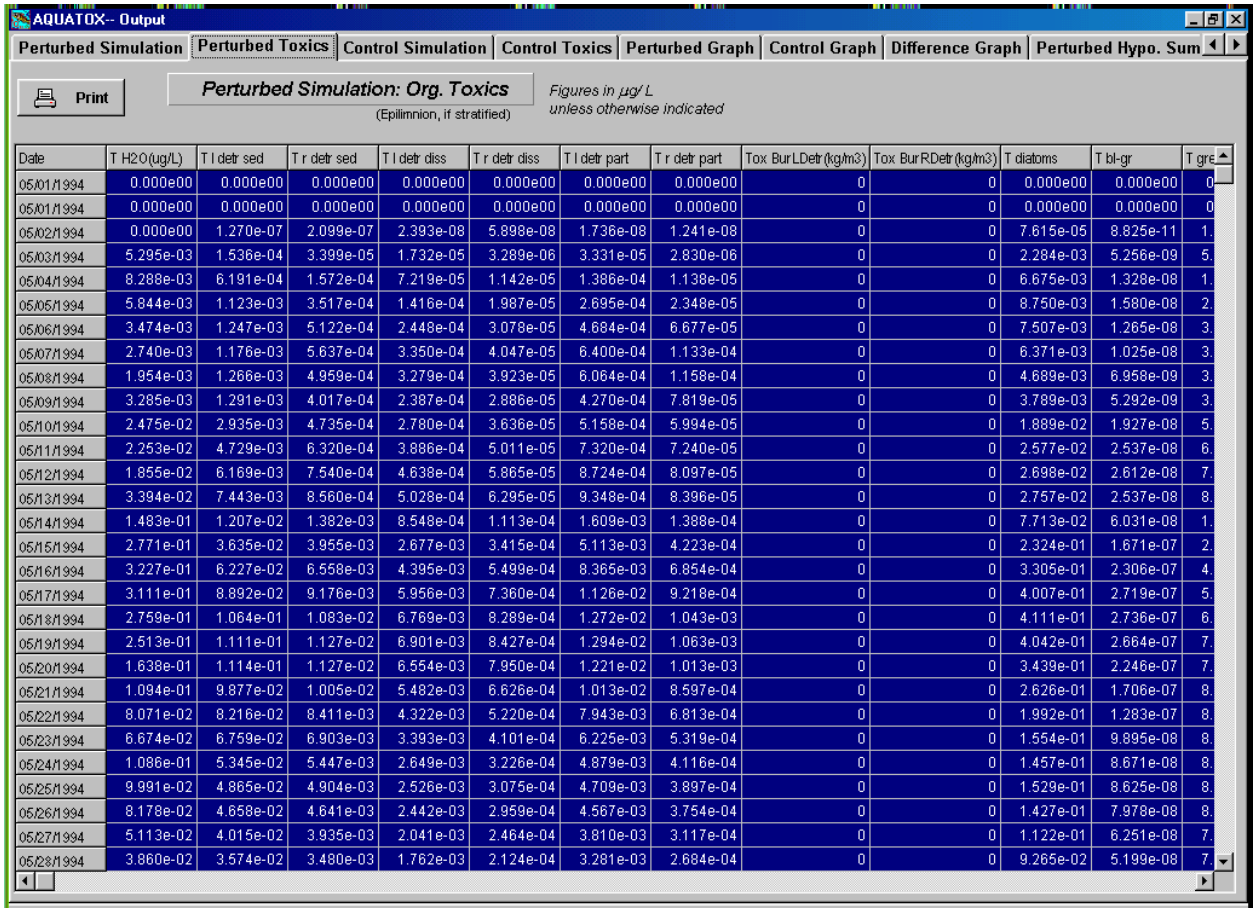
Date	T H2O(ug/L)	NH4	NO3	PO4	CO2	Oxygen	L detr sed(g/m2)	R detr sed(g/m2)	L detr diss	R detr diss	L detr part	R detr part
05/01/1994	0.000e00	0.08	0.05	0.05	1.5	12	3	3	0.18	0.72	0.02	0.08
05/01/1994	0.000e00	0.08	0.05	0.05	1.5	12	3	3	0.18	0.72	0.02	0.08
05/02/1994	0.000e00	0.03484	16.61757	1.66579	0.66017	11.26169	2.00224	3.49875	0.34843	0.81714	0.26875	0.18113
05/03/1994	5.295e-03	0.01636	39.18504	3.87087	0.51843	11.06612	1.79559	3.8987	0.46168	0.80451	0.4975	0.16973
05/04/1994	8.288e-03	0.01382	55.6873	5.48552	0.52874	11.14057	2.07042	4.28848	0.5667	0.79795	0.68842	0.16728
05/05/1994	5.844e-03	0.01416	71.46411	7.03016	0.53175	11.27855	2.75449	5.29644	0.71517	0.79751	0.94987	0.18569
05/06/1994	3.474e-03	0.01812	87.71544	8.62348	0.56928	11.3406	3.43018	6.69616	1.17883	0.83227	1.81318	0.35658
05/07/1994	2.740e-03	0.02336	98.32999	9.66712	0.60436	11.29634	3.88853	7.77641	1.64109	0.87368	2.64127	0.53952
05/08/1994	1.954e-03	0.03384	116.34827	11.44486	0.65152	11.17536	5.76211	9.01132	2.11928	0.9132	3.30516	0.67477
05/09/1994	3.285e-03	0.04139	129.30343	12.72666	0.6845	11.11547	7.70029	9.50511	2.25412	0.91938	3.33483	0.66388
05/10/1994	2.475e-02	0.05549	153.78817	15.15563	0.75664	11.09421	11.71028	10.16647	2.39652	0.92036	3.20118	0.59877
05/11/1994	2.253e-02	0.0621	165.10802	16.28128	0.79278	11.11382	13.63695	10.41307	2.44945	0.92155	3.13522	0.56906
05/12/1994	1.855e-02	0.0687	175.51116	17.31734	0.83236	11.15076	15.42586	10.61504	2.49227	0.92012	3.07893	0.54101
05/13/1994	3.394e-02	0.07975	192.61292	19.02387	0.90005	11.22271	18.40711	10.91536	2.56099	0.91799	3.00802	0.49979
05/14/1994	1.483e-01	0.09205	210.37632	20.80114	0.9784	11.30833	21.5414	11.19615	2.63191	0.91624	2.96311	0.46375
05/15/1994	2.771e-01	0.10609	230.16095	22.78685	1.07291	11.39932	25.07285	11.48622	2.71427	0.91538	2.94705	0.43161
05/16/1994	3.227e-01	0.11603	243.96301	24.1766	1.13908	11.43418	27.55866	11.68009	2.77485	0.91561	2.95482	0.41378
05/17/1994	3.111e-01	0.1267	258.42419	25.63742	1.20823	11.43194	30.17467	11.87814	2.84064	0.91656	2.97649	0.39865
05/18/1994	2.759e-01	0.13702	272.11895	27.02606	1.27214	11.38466	32.65566	12.0623	2.90462	0.91807	3.00721	0.38728
05/19/1994	2.513e-01	0.14195	278.62171	27.68747	1.30266	11.34634	33.81377	12.14372	2.93564	0.91902	3.0251	0.38288
05/20/1994	1.638e-01	0.15273	292.87273	29.14207	1.36689	11.23062	36.28513	12.33979	3.00728	0.92186	3.07552	0.37652
05/21/1994	1.094e-01	0.16388	307.82946	30.67723	1.42674	11.07062	38.80516	12.60002	3.08796	0.92602	3.1439	0.37473
05/22/1994	8.071e-02	0.17406	321.43157	32.08212	1.47905	10.88986	41.0325	12.82407	3.15965	0.93013	3.20504	0.37419
05/23/1994	6.674e-02	0.18319	333.32015	33.31787	1.52052	10.71855	43.11605	13.04723	3.24363	0.96226	3.27382	0.39856
05/24/1994	1.086e-01	0.19539	349.47219	35.00909	1.57587	10.49373	45.91223	13.25844	3.31011	0.96518	3.31673	0.39014
05/25/1994	9.991e-02	0.20681	364.65396	36.61249	1.62955	10.29279	48.5017	13.41617	3.36681	0.96781	3.35131	0.38301
05/26/1994	8.178e-02	0.21451	374.56108	37.66659	1.6669	10.16134	50.16686	13.50738	3.40071	0.96944	3.37144	0.37891
05/27/1994	5.113e-02	0.22949	394.42465	39.79891	1.74057	9.92095	53.4181	13.66197	3.4629	0.97265	3.40818	0.37206
05/28/1994	3.860e-02	0.23638	403.89774	40.82538	1.77337	9.81235	54.91734	13.724	3.4895	0.9741	3.4237	0.36937

The **Control Simulation** presents the results of a simulation without the perturbation. In this way even subtle, indirect effects can be discerned. Furthermore, comparison of perturbed and control runs ensures that consistent evaluations are obtained without undue concern with how well calibrated the model is for a particular site.



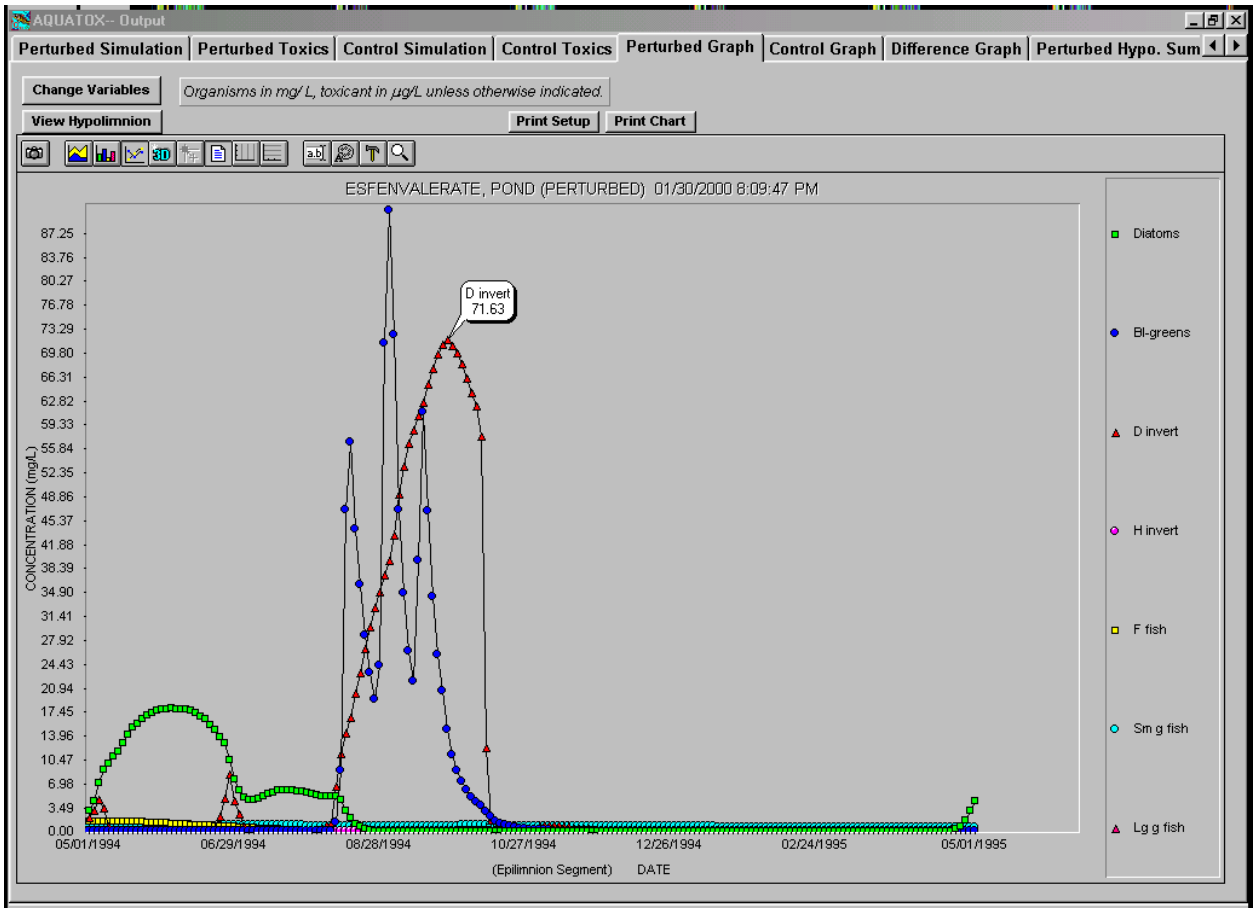
Date	T H2O(ug/L)	NH4	NO3	PO4	CO2	Oxygen	L detr sed(g/m2)	R detr sed(g/m2)	L detr diss	R detr diss	L detr part	R detr part
05/01/1994	0	0.08	0.05	0.05	1.5	12	3	3	0.18	0.72	0.02	0.08
05/01/1994	0	0.08	0.05	0.05	1.5	12	3	3	0.18	0.72	0.02	0.08
05/02/1994	0	0.03484	16.61757	1.66579	0.66017	11.26169	2.00224	3.49875	0.34843	0.81714	0.26875	0.18113
05/03/1994	0	0.01447	48.54497	4.78639	0.52519	11.0967	1.89745	4.06794	0.51873	0.80037	0.60326	0.1676
05/04/1994	0	0.01444	64.62602	6.35989	0.55808	11.1929	2.17196	4.39216	0.62943	0.79513	0.79555	0.16714
05/05/1994	0	0.01646	80.56893	7.91961	0.60196	11.29753	2.5011	4.7629	0.75332	0.79201	0.99609	0.17012
05/06/1994	0	0.01942	96.38253	9.46638	0.64983	11.38096	2.84478	5.17955	0.88753	0.79035	1.20031	0.17544
05/07/1994	0	0.02285	112.06991	11.00106	0.69893	11.43713	3.18453	5.63688	1.02978	0.79026	1.40444	0.18285
05/08/1994	0	0.02653	127.63151	12.52438	0.74815	11.47296	3.51072	6.12657	1.17738	0.79149	1.60466	0.19179
05/09/1994	0	0.03035	143.06686	14.03698	0.79728	11.50046	3.81877	6.63907	1.32782	0.79383	1.79775	0.20177
05/10/1994	0	0.03424	158.37544	15.53934	0.84666	11.53055	4.10886	7.16673	1.48051	0.79879	1.98289	0.21406
05/11/1994	0	0.03818	173.55706	17.03189	0.89679	11.56941	4.37997	7.70054	1.63332	0.8061	2.158	0.22798
05/12/1994	0	0.04209	188.61176	18.51491	0.94752	11.61929	4.62914	8.22481	1.77952	0.81042	2.3171	0.2383
05/13/1994	0	0.04594	203.53976	19.98862	0.99876	11.67609	4.86324	8.73564	1.92144	0.81514	2.46356	0.2486
05/14/1994	0	0.0496	218.34108	21.45321	1.04919	11.73159	5.08375	9.22775	2.05875	0.82027	2.59812	0.25875
05/15/1994	0	0.05302	233.01516	22.90882	1.09805	11.77403	5.29231	9.69733	2.19145	0.8258	2.72185	0.26869
05/16/1994	0	0.05629	247.56076	24.35566	1.14468	11.79077	5.48983	10.14008	2.31911	0.83167	2.83526	0.27834
05/17/1994	0	0.05944	261.97577	25.79391	1.18837	11.77148	5.67715	10.55243	2.44125	0.83779	2.9388	0.28764
05/18/1994	0	0.06249	276.25715	27.22376	1.2285	11.71062	5.85483	10.93168	2.55753	0.84409	3.03295	0.29655
05/19/1994	0	0.06543	290.40117	28.64539	1.26487	11.60893	6.02321	11.27586	2.66766	0.85049	3.11821	0.30503
05/20/1994	0	0.06827	304.40376	30.05895	1.29777	11.47337	6.18248	11.58369	2.77143	0.85693	3.19507	0.31308
05/21/1994	0	0.07094	318.26114	31.46458	1.32598	11.31786	6.3266	11.86128	2.86863	0.86335	3.26382	0.32062
05/22/1994	0	0.07321	331.97088	32.8624	1.34418	11.16513	6.43383	12.14129	2.9587	0.86963	3.324	0.32744
05/23/1994	0	0.07517	345.53207	34.25254	1.35839	11.02233	6.51925	12.42292	3.04145	0.87572	3.37593	0.33352
05/24/1994	0	0.07693	358.94465	35.63513	1.37144	10.89341	6.5916	12.70217	3.11689	0.88154	3.42011	0.3389
05/25/1994	0	0.07854	372.2093	37.01025	1.38427	10.77964	6.65444	12.97684	3.18506	0.88707	3.45707	0.3436
05/26/1994	0	0.08002	385.3271	38.378	1.39694	10.6793	6.70949	13.24564	3.2461	0.89226	3.48737	0.34767
05/27/1994	0	0.0814	398.29912	39.73848	1.40914	10.58862	6.75773	13.50779	3.30017	0.89709	3.51156	0.35114
05/28/1994	0	0.08268	411.12617	41.09179	1.42043	10.50334	6.79976	13.76286	3.34749	0.90153	3.53016	0.35406

The **Perturbed Toxics** and **Control Toxics** tables give masses of toxicant associated with each compartment or carrier (in µg/L, mass per unit volume) , total mass, time-varying half-lives (in days), concentrations (in µg/kg, ppb), and rates of degradation, volatilization, and loadings (in µg/L-d).



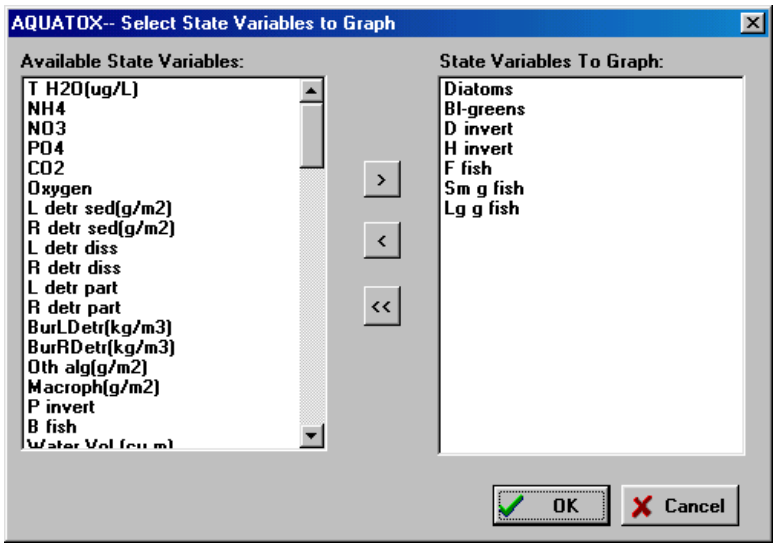
Date	T H2O (ug/L)	T l detr sed	T r detr sed	T l detr diss	T r detr diss	T l detr part	T r detr part	Tox BurLDetr (kg/m3)	Tox BurRDetr (kg/m3)	T diatoms	T bl-gr	T gre
05/01/1994	0.000e00	0.000e00	0.000e00	0.000e00	0.000e00	0.000e00	0.000e00	0	0	0.000e00	0.000e00	0
05/01/1994	0.000e00	0.000e00	0.000e00	0.000e00	0.000e00	0.000e00	0.000e00	0	0	0.000e00	0.000e00	0
05/02/1994	0.000e00	1.270e-07	2.099e-07	2.393e-08	5.898e-08	1.736e-08	1.241e-08	0	0	7.615e-05	8.825e-11	1.
05/03/1994	5.295e-03	1.536e-04	3.399e-05	1.732e-05	3.289e-06	3.331e-05	2.830e-06	0	0	2.284e-03	5.256e-09	5.
05/04/1994	8.288e-03	6.191e-04	1.572e-04	7.219e-05	1.142e-05	1.386e-04	1.138e-05	0	0	6.675e-03	1.328e-08	1.
05/05/1994	5.844e-03	1.123e-03	3.517e-04	1.416e-04	1.987e-05	2.695e-04	2.348e-05	0	0	8.750e-03	1.580e-08	2.
05/06/1994	3.474e-03	1.247e-03	5.122e-04	2.448e-04	3.078e-05	4.684e-04	6.677e-05	0	0	7.507e-03	1.265e-08	3.
05/07/1994	2.740e-03	1.176e-03	5.637e-04	3.350e-04	4.047e-05	6.400e-04	1.133e-04	0	0	6.371e-03	1.025e-08	3.
05/08/1994	1.954e-03	1.266e-03	4.959e-04	3.279e-04	3.923e-05	6.064e-04	1.158e-04	0	0	4.689e-03	6.958e-09	3.
05/09/1994	3.285e-03	1.291e-03	4.017e-04	2.387e-04	2.886e-05	4.270e-04	7.819e-05	0	0	3.789e-03	5.292e-09	3.
05/10/1994	2.475e-02	2.935e-03	4.735e-04	2.780e-04	3.636e-05	5.158e-04	5.994e-05	0	0	1.889e-02	1.927e-08	5.
05/11/1994	2.253e-02	4.729e-03	6.320e-04	3.886e-04	5.011e-05	7.320e-04	7.240e-05	0	0	2.577e-02	2.537e-08	6.
05/12/1994	1.855e-02	6.169e-03	7.540e-04	4.638e-04	5.865e-05	8.724e-04	8.097e-05	0	0	2.698e-02	2.612e-08	7.
05/13/1994	3.394e-02	7.443e-03	8.560e-04	5.028e-04	6.295e-05	9.348e-04	8.396e-05	0	0	2.757e-02	2.537e-08	8.
05/14/1994	1.483e-01	1.207e-02	1.382e-03	8.548e-04	1.113e-04	1.609e-03	1.388e-04	0	0	7.713e-02	6.031e-08	1.
05/15/1994	2.771e-01	3.635e-02	3.955e-03	2.677e-03	3.415e-04	5.113e-03	4.223e-04	0	0	2.324e-01	1.671e-07	2.
05/16/1994	3.227e-01	6.227e-02	6.558e-03	4.395e-03	5.499e-04	8.365e-03	6.854e-04	0	0	3.305e-01	2.306e-07	4.
05/17/1994	3.111e-01	8.892e-02	9.176e-03	5.956e-03	7.360e-04	1.126e-02	9.218e-04	0	0	4.007e-01	2.719e-07	5.
05/18/1994	2.759e-01	1.064e-01	1.083e-02	6.769e-03	8.289e-04	1.272e-02	1.043e-03	0	0	4.111e-01	2.736e-07	6.
05/19/1994	2.513e-01	1.111e-01	1.127e-02	6.901e-03	8.427e-04	1.294e-02	1.063e-03	0	0	4.042e-01	2.664e-07	7.
05/20/1994	1.638e-01	1.114e-01	1.127e-02	6.554e-03	7.950e-04	1.221e-02	1.013e-03	0	0	3.439e-01	2.246e-07	7.
05/21/1994	1.094e-01	9.877e-02	1.005e-02	5.482e-03	6.626e-04	1.013e-02	8.597e-04	0	0	2.626e-01	1.706e-07	8.
05/22/1994	8.071e-02	8.216e-02	8.411e-03	4.322e-03	5.220e-04	7.943e-03	6.813e-04	0	0	1.992e-01	1.283e-07	8.
05/23/1994	6.674e-02	6.759e-02	6.903e-03	3.393e-03	4.101e-04	6.225e-03	5.319e-04	0	0	1.554e-01	9.895e-08	8.
05/24/1994	1.086e-01	5.345e-02	5.447e-03	2.649e-03	3.226e-04	4.879e-03	4.116e-04	0	0	1.457e-01	8.671e-08	8.
05/25/1994	9.991e-02	4.865e-02	4.904e-03	2.526e-03	3.075e-04	4.709e-03	3.897e-04	0	0	1.529e-01	8.625e-08	8.
05/26/1994	8.178e-02	4.658e-02	4.641e-03	2.442e-03	2.959e-04	4.567e-03	3.754e-04	0	0	1.427e-01	7.978e-08	8.
05/27/1994	5.113e-02	4.015e-02	3.935e-03	2.041e-03	2.464e-04	3.810e-03	3.117e-04	0	0	1.122e-01	6.251e-08	7.
05/28/1994	3.860e-02	3.574e-02	3.480e-03	1.762e-03	2.124e-04	3.281e-03	2.684e-04	0	0	9.265e-02	5.199e-08	7.

Graph—Limited graphing capability also is available. Click on the **Perturbed Graph** tab and you will get a default graph for the perturbed simulation with representative ecologic guilds. By double-clicking on a given point on a line you will get label for the line and value for the particular point.

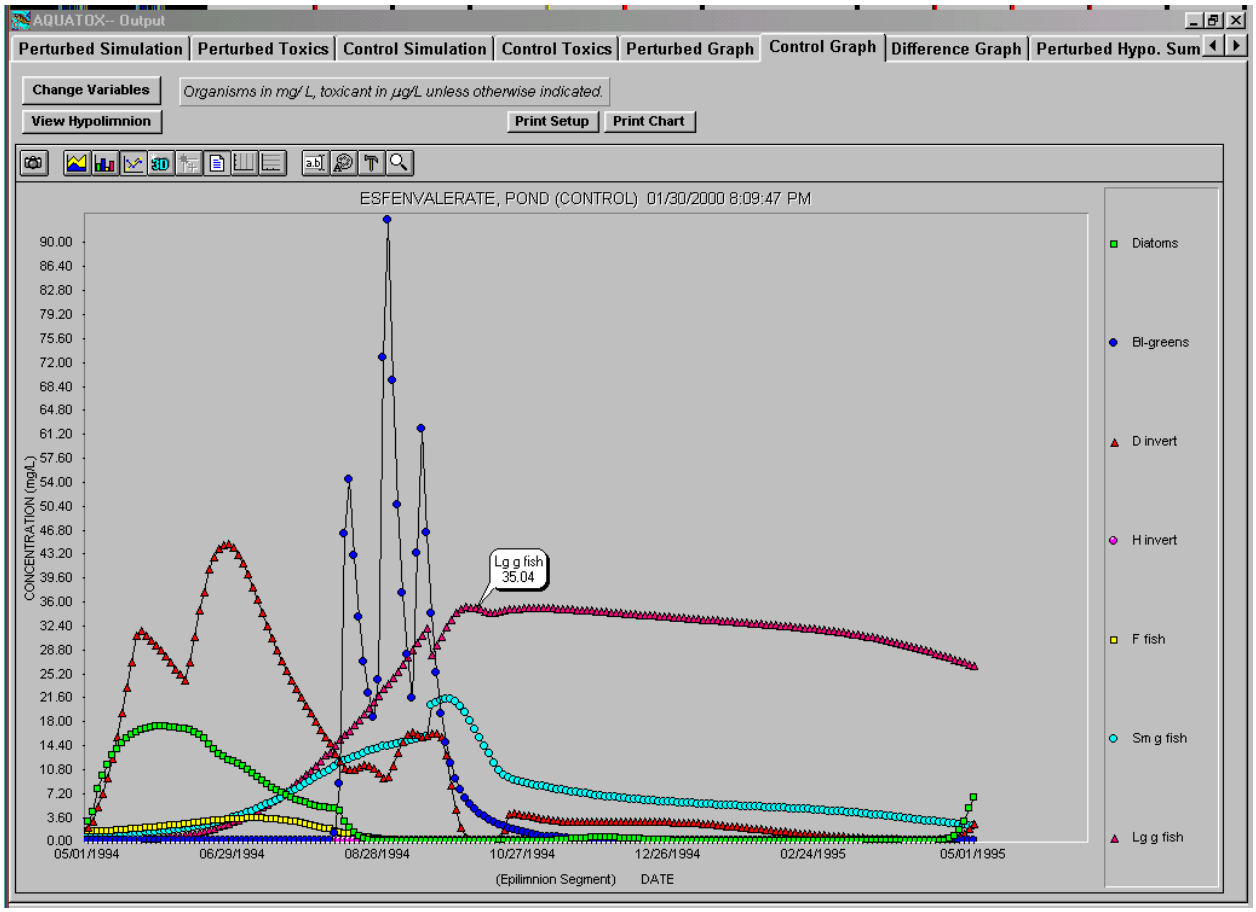


The color of the lines and symbols can be changed by clicking on the hammer (tool) icon and selecting **Palette Bar**. The color can be dragged to the line (the cursor becomes a fill symbol to indicate the procedure). Be careful that the fill symbol is on a line and not on the background, or you will change the background! The scale can be changed by clicking on the magnifying glass icon, and changing the maximum scale value. The titles and axis labels can be changed by clicking on the icon labeled "ab" and changing the appropriate text.

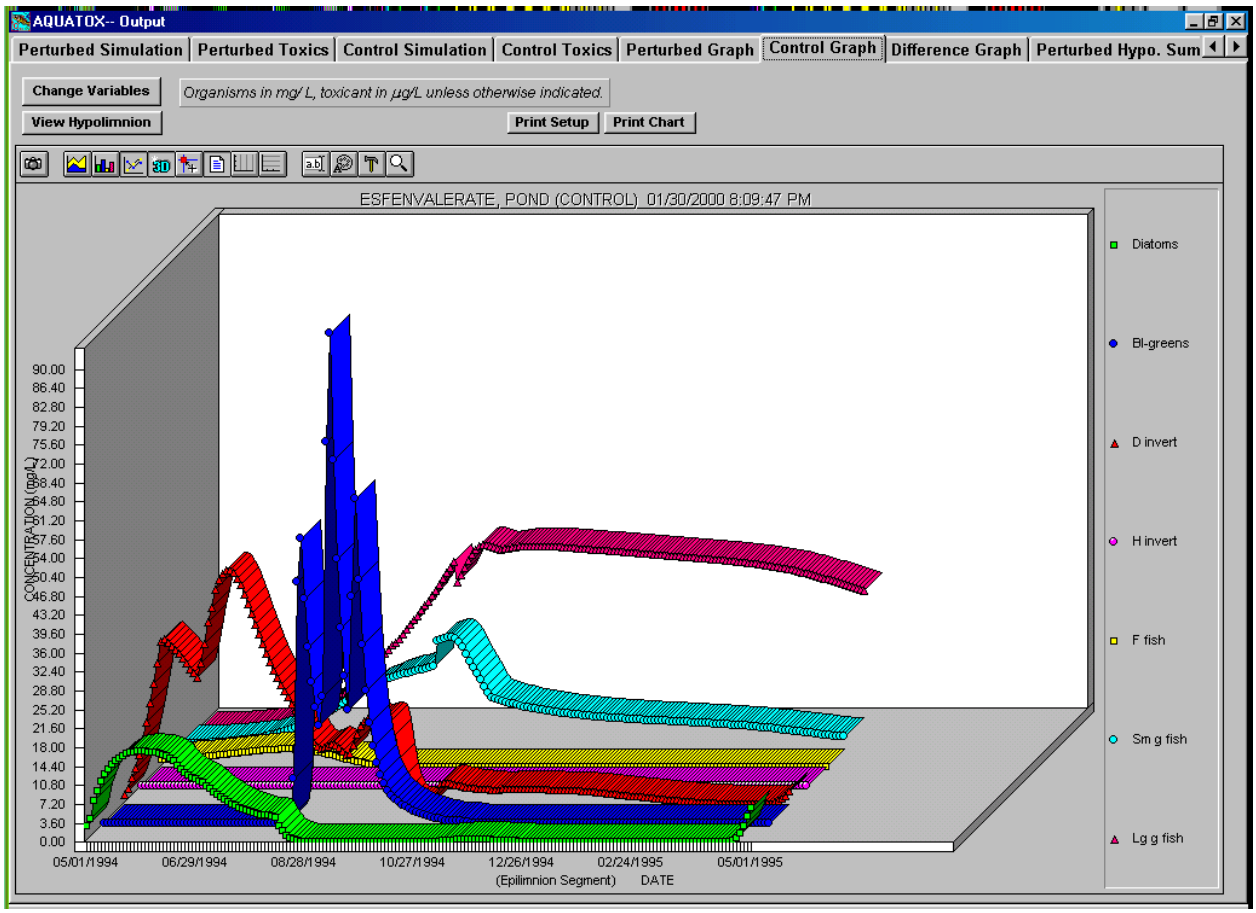
You will probably wish to change the state variables plotted, so click on the **Change Variables** button on the upper left. You can highlight one compartment, or you can highlight several choices in the list on the left at once by highlighting the top one, moving the cursor down, and pressing the shift key and the mouse button together. Clicking on the ▶ symbol will move the choices to the window on the right. By clicking on the ▯ symbol you clear the list on the right.



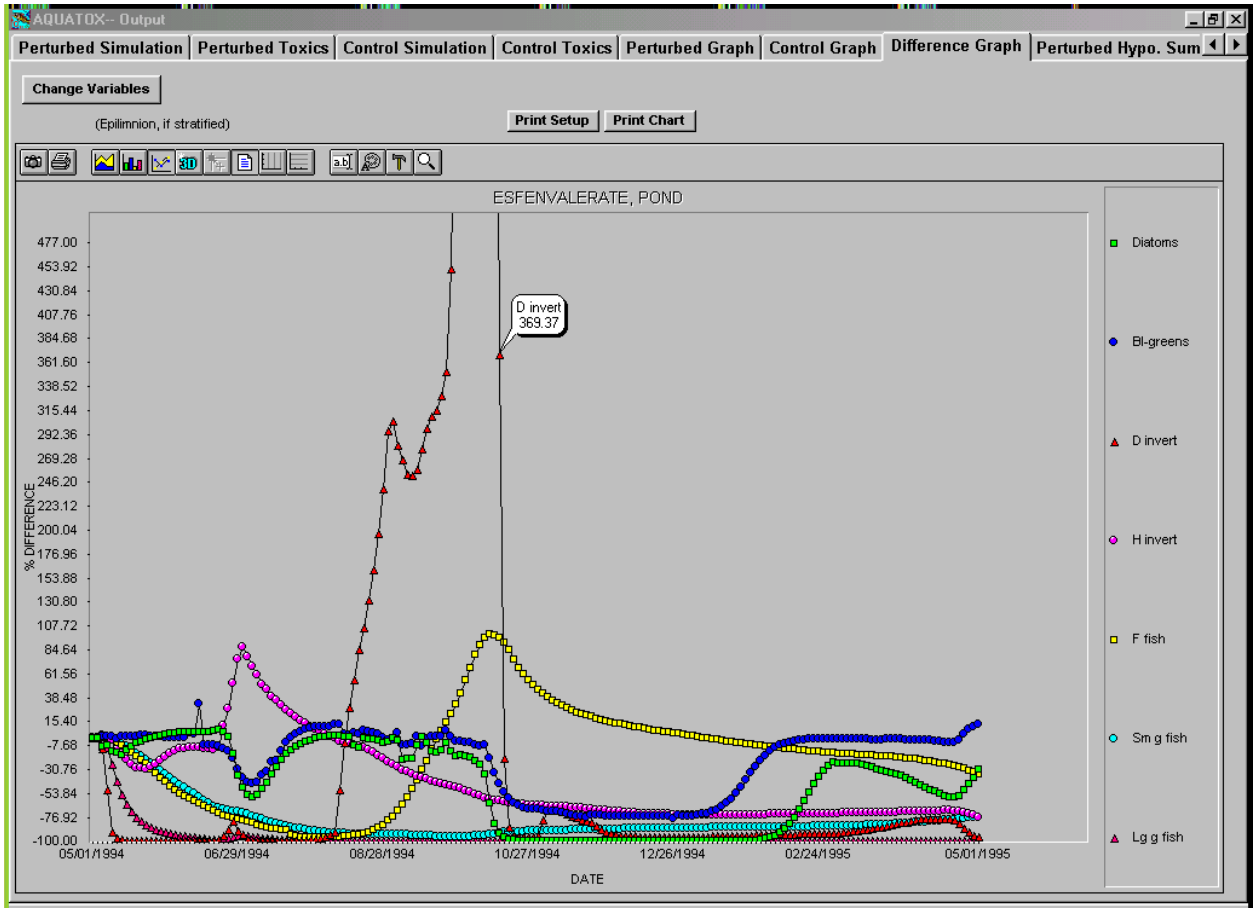
Click on the **Control Graph** tab, and you will get a comparable plot of the control simulation.



By clicking on the **3D** icon you can get a ribbon graph. Another option is an area graph. "A picture is worth a thousand words," so experiment with the other icons.



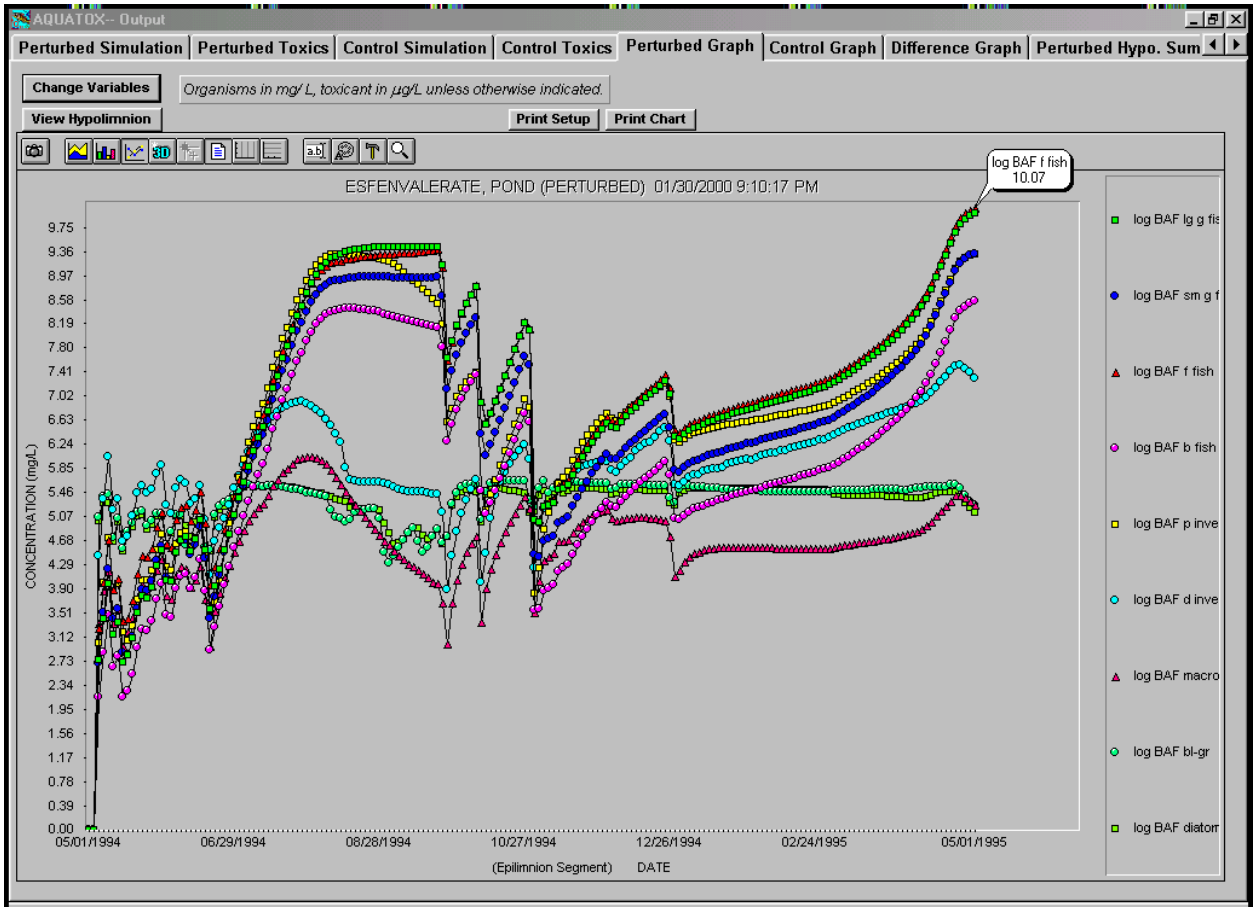
More informative is the **Difference Graph**, which plots the percent difference of the Perturbed minus the Control values for the state variables. It is an excellent way to isolate and portray the direct and indirect effects of the perturbation. For example, in the pond study most animals were affected by chronic and acute toxicity to esfenvalerate. However, the detritivorous invertebrates (amphipods) recovered quickly. The forage fish (bluegill) rebounded in part due to the abundant amphipods and benefitted from decreased predation from the large game fish (bass), which did not fully recover during the year-long simulation.



A graph can be printed by clicking on the **Print** button. **Print Setup** allows you to specify the printer and its properties. You also can save the graph to the Windows Clipboard by clicking on the camera icon. If you wish better graphics, then you should export results to a file to be processed by a spreadsheet program.

The model also can compute and plot or tabulate lipid-normalized bioaccumulation factors (BAFs). Two methods are provided for the computation: the actual BAF based on a comparison of the concentrations in the organisms and the concentration in the truly dissolved phase in the water, and a computation based on a "dissolved" concentration that includes dissolved and complexed to dissolved organic matter—the latter for comparison with older literature values that did not account for complexed contaminant. The choice of computational method may be made in the **Setup** screen. If you choose "Log BAF" from the list of available variables, the resulting plot shows that

esfenvalerate has a log BAF over 10 in forage fish (bluegill) at the end of the simulation, indicating that is a highly bioaccumulative chemical, especially in a complex food web.



Files—You may wish to export the files for use in another program. From the **Study Information** screen, click on **Export Results**, to export the results of the simulation with the toxicant, or **Export Control**. The default will be in dBase *dbf* format, which is limited to eight upper-case letters in the column headings. The full headings will be exported if you choose Paradox *db* format, which is the native format of the AQUATOX data structures. A third option is to export as delimited ASCII files suitable for importing into almost any spreadsheet.

Note that the library databases, saved in the Database subdirectory, also are in Paradox format. To read and edit them with a Paradox-compatible program it is necessary to rename them with a *db* extension, instead of *sdb*, *cdb*, *pdb*, or *adb* for site, chemical, plant, and animal databases. Don't forget to change the extension back before attempting to use it with AQUATOX.

3. APPLICATIONS

The following examples are intended as illustrations of potential applications. AQUATOX has been validated with several data sets from diverse sites and applications; however, like any complex model, it should be evaluated for the intended use. More detailed reports on model validation, including analysis of model predictions as compared to observed data, are found in **Volume 3: Model Validation Reports**. No warranty, either expressed or implied, is made.

3.1 Nutrient Enrichment

AQUATOX has its roots in what was basically a eutrophication model, and it provides a reasonable representation of the effects of nutrient enrichment. It can be configured to depict a complex food web that is both phytoplankton- and detritus-based, with both game fish and bottom fish, which are very important from the standpoint of protecting aquatic life and fisheries. It also reports phytoplankton both as biomass and as chlorophyll *a*, which is an important index of water quality. Dissolved oxygen is another important index that is computed. The Secchi depth, an indicator of clarity, also is estimated.

For our first example, we will use data from Onondaga Lake, New York (*Onondaga.aps*). The lake has been described very well in a book edited by Effler (1996). It has received municipal and industrial wastes for many years, and effluent from the municipal wastewater treatment plant accounts for nearly 20% of the annual inflow to the lake (Effler, 1996). Of particular concern are the combined sewer overflows (CSOs) that carry storm water and raw sewage into tributary creeks about 50 times a year. In 1991 there were 45 CSOs discharging into Onondaga Creek, 19 into Harbor Brook, and 2 into Ley Creek. In a separate report, Park (1999b) described three levels of analyses in validating Version 1.66 with Onondaga Lake data. For purposes of this example, we will use the third-level implementation with detailed loadings for nutrients, a site-specific mixing depth, and compartments parameterized for cryptomonads and rotifers.

Discharge data from the four gauged streams in the watershed (Onondaga Creek, Ninemile Creek, Ley Creek, and Harbor Brook, listed in order of importance) were downloaded from the U.S. Geological Survey Web site (see Table 1). Discharge from four ungauged streams was estimated, assuming that they had an aggregate flow rate that was 94% of the discharge of Ley Creek and Harbor Brook based on data in Effler (1996, p. 102).

Table 1. Input Data for Onondaga Lake Simulation

Variable	Source	Format
Inflow	www.waterdata.usgs.gov (note: URLs may change)	daily values for 4 gauged streams; extrapolated to ungauged streams
Phosphorus, NPS	Effler 1996, calc. from p. 162 Effler 1996, calc. from p. 159	mean annual conc., 7 tributaries, 1989-1990; mult. by respective inflow
METRO	Effler 1996, p. 162	mean loads, April-September, 1990
NO_x & NH_3, NPS	Effler 1996, calc. from p. 138 Effler 1996, calc. from p. 128	mean annual concentrations for 1989 for 4 tributaries
METRO	Effler 1996, calc. from p. 138	mean annual loads for 1989
Org. matter, NPS	Effler 1996, calc. from p. 138 Effler 1996, calc. from p. 128	back-calculated from organic-N
METRO	Effler 1996, calc. from p. 138	mean annual loads for 1989
Epilimnion temperature	Effler 1996, p. 207	monthly interpolation from figure
Hypolimnion temperature	Effler 1996, p. 247	monthly interpolation from figure
Wind	Effler 1996, p. 248	mean value est. from figure for 30 years
Solar radiation	unpub. data, Lake George, N.Y.	observed annual mean and range
Initial conditions	Effler 1996	obs. data and professional judgment

The loadings were then computed using average concentrations for the respective streams, assuming a constant relationship between concentration and discharge. Different average phosphate values were used for 1989 and 1990 for Onondaga and Ninemile Creeks, which varied considerably between the two years due to combined sewer overflows. Also, the concentration of ammonia in Ninemile Creek, which flows through soda ash waste beds, exhibits an inverse relationship to flow rate according to Effler (1996, p. 131); therefore, his Equation 3.12 was used to compute the ammonia concentrations:

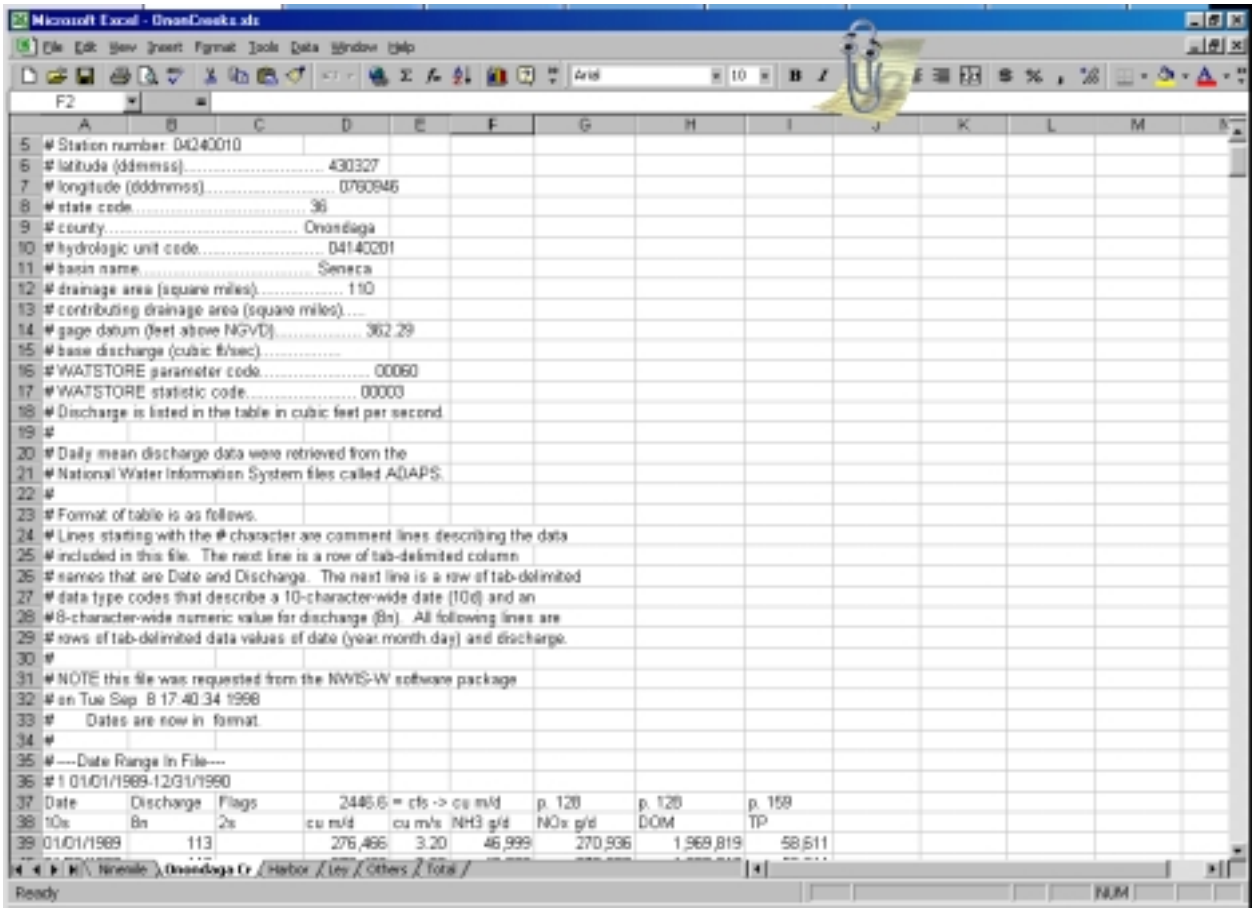
$$[T\text{-}NH_3] = 0.20 + \frac{0.73}{Flow}$$

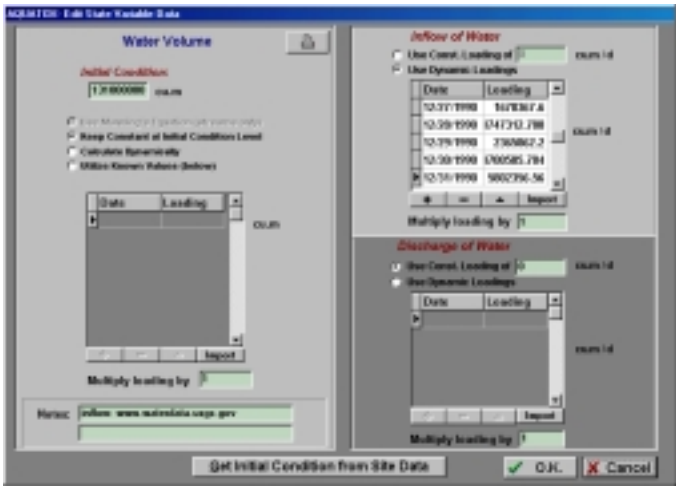
where:

$[T\text{-}NH_3]$ = concentration of total ammonia (mgN/L),

Flow = flow rate (m^3/s).

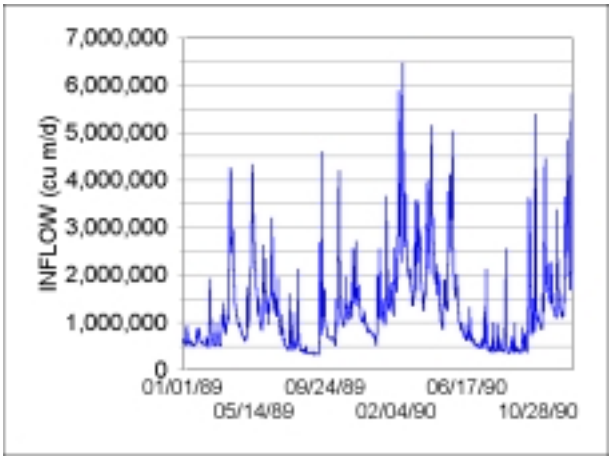
The computations were performed in a spreadsheet by first converting the discharge data from cfs to m^3/d and m^3/s then, for the nutrients, multiplying by the given concentrations to obtain mass per day (g/d) in successive columns. The loadings were imported into AQUATOX by clicking on **Import** in the Edit State Variable screen and choosing the appropriate comma-delimited (csv) or database file.



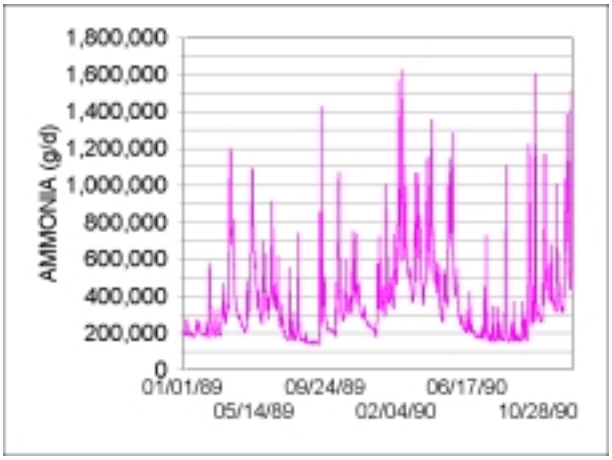


Given the readily available hydrologic data, both 1989 and 1990 were simulated with daily loadings. Examination of the loading plots confirms that the streams draining into Onondaga Lake are indeed "flashy" or subject to fast runoff with distinct peaks; the nutrient and organic matter loadings vary accordingly, except the ammonia loadings, which vary slightly from the other loadings due to the inverse flow relationship cited above. The data files and plots were prepared using Quattro Pro and Excel.

Onondaga Lake inflow



Onondaga Lake ammonia loadings



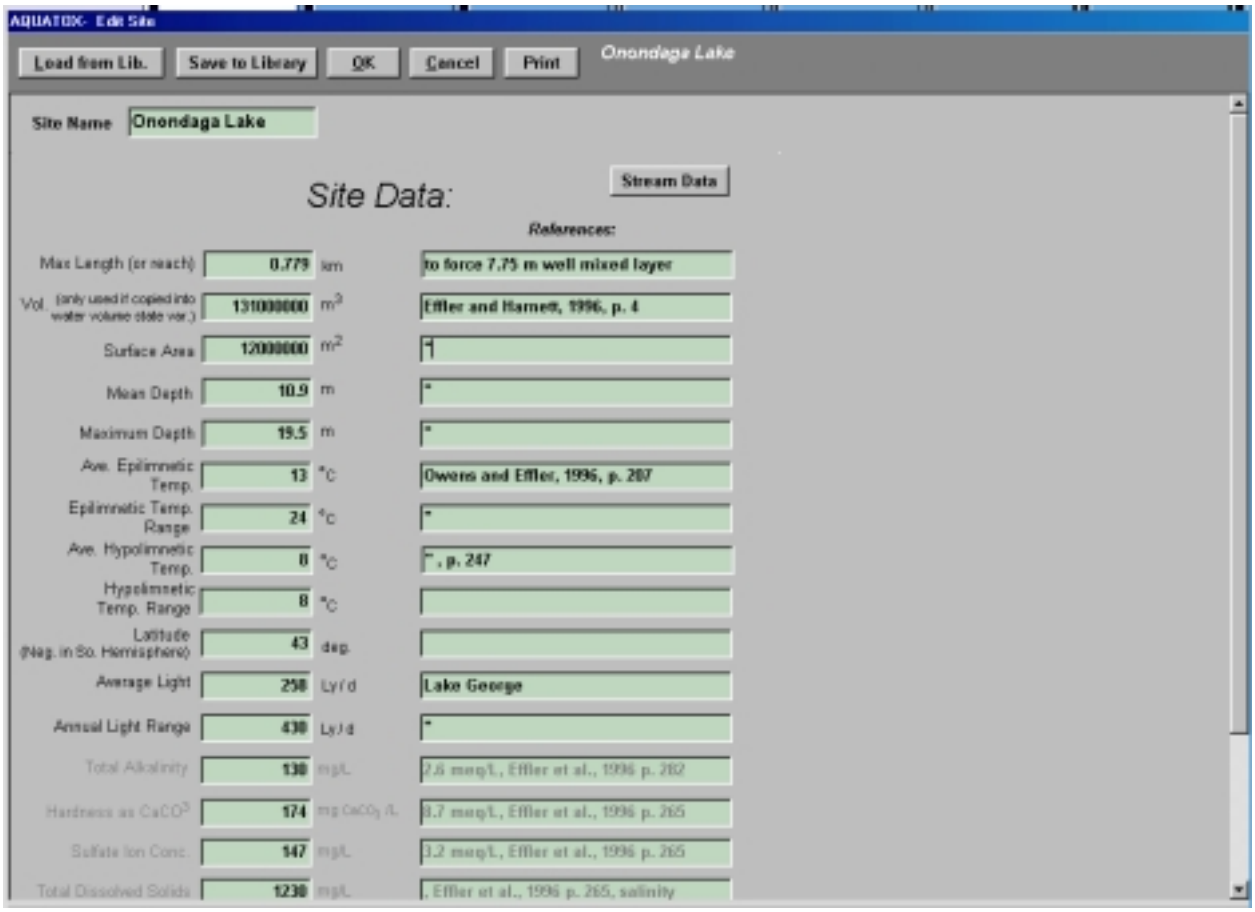
Results from preliminary model runs indicated that some of the model assumptions and defaults were inappropriate for this application, and therefore needed to be modified. For instance, the model computes the depth of the well mixed layer (epilimnion) using a robust regression equation with the fetch (distance across which the wind can blow) as the independent variable; this equation is based on a dataset for 167 lakes. In Onondaga Lake the computed mixing depth of 15 m is twice as deep as observed (Effler, 1996). It appears that salinity from industrial pollution in the lake is restricting the mixing depth. By back-calculating from the regression equation, a fetch (*Length*) of 0.779 km was found to give the observed well mixed depth (*MaxZMix*) of 7.75 m:

$$MaxZMix = Length^{0.336} \cdot 0.569$$

$$\log(Length) = \frac{\log(7.75)}{0.336} + 0.245$$

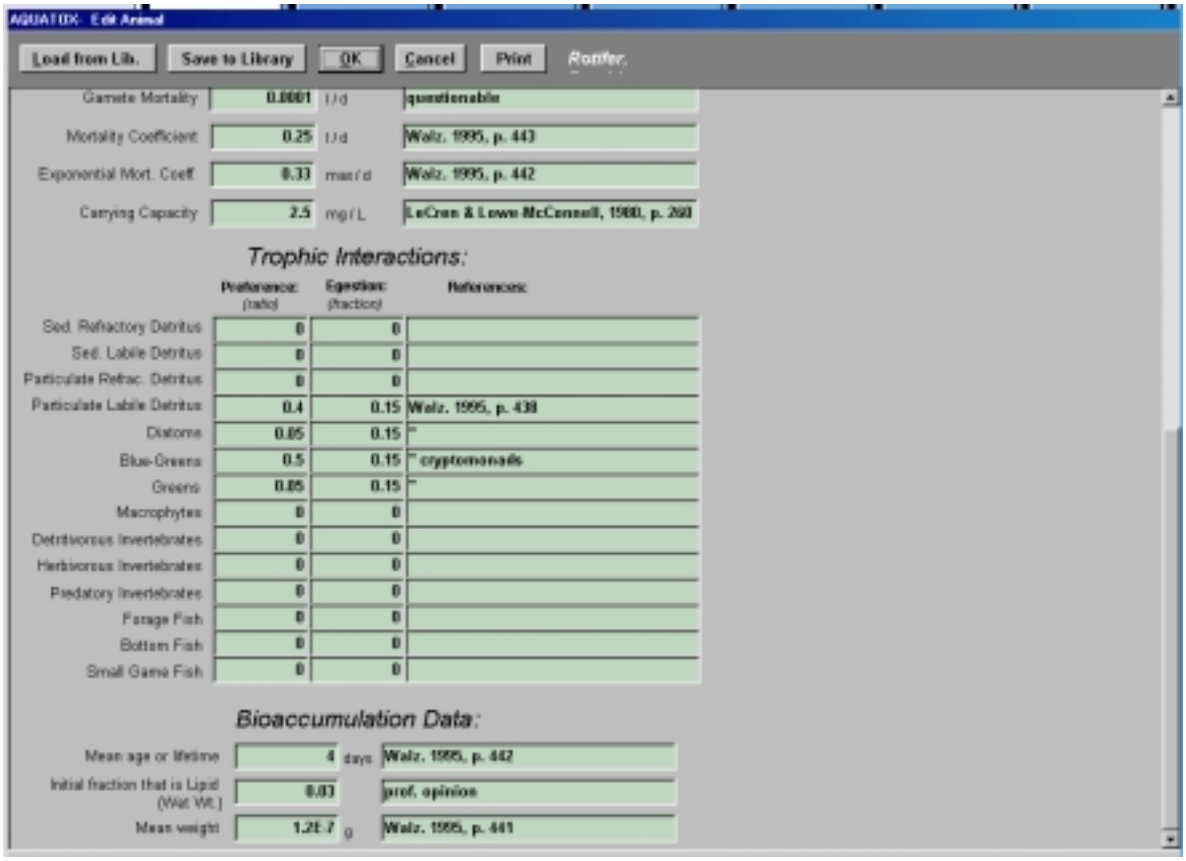
$$Length = 779 \text{ m}$$

The maximum length was then changed in the Site Characteristics screen.

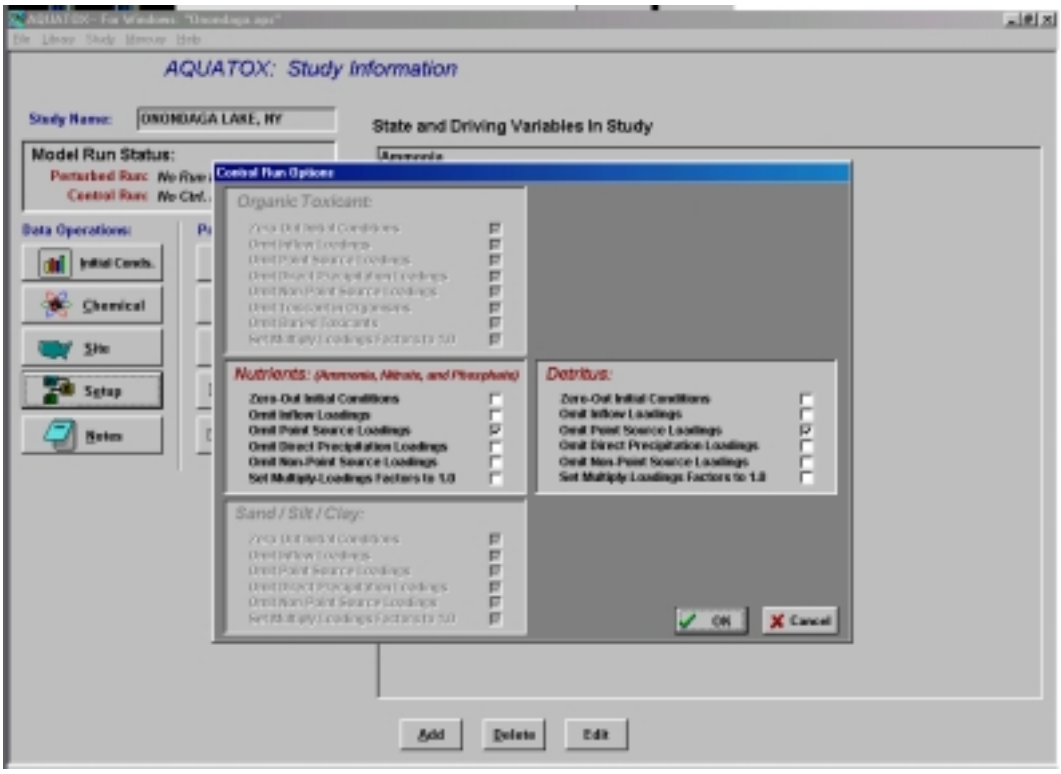


A second modification was necessary because the observed spring algal bloom was not predicted in initial runs. The spring bloom was reported to be due to cryptomonads, a flagellated algal group that was not in the default data set. Using values from Collins and Wlosinski (1983), a cryptomonad compartment was parameterized. The present version of AQUATOX can simulate three algal groups; diatoms and green algae are more important than blue-greens in Onondaga Lake, so cryptomonads were substituted for blue-greens. This is appropriate because the model assumes that blue-greens occupy the top meter of water unless the wind exceeds 3 m/s, when Langmuir stripes form, and cryptomonads also tend to move toward the surface. Rotifers are important grazers on cryptomonads, and predatory zooplankton probably are unimportant in the lake, so rotifers were substituted for predatory zooplankton. Furthermore, the food preferences for rotifers were changed to force them to "eat" cryptomonads in the model.


AQUATOX: Edit Animal
Load from Lib.
Save to Library
OK
Cancel
Print
Rotifer.
Animal: Rotifer, Brachionus
Animal Type: Pelagic Invert.
Toxicity Record: Daphnia
Animal Data:
References:
Half Saturation Feeding 1 mg/L Walz, 1995, p. 441
Maximum Consumption 3.438 g/g-d Collins & Wlosinski 1983, p. 45
Min Prey for Feeding 0.6 mg/L Walz, 1995, p. 441
Temp. Response Slope 2 default
Optimum Temperature 25 °C Walz, 1995, p. 443
Maximum Temperature 35 °C prof. opinion
Min Adaptation Temp. 2 °C cold-adapted (see Walz, 1995)
Respiration Rate 0.34 1/d Leidy & Ploskey, 1980, p. 020
Specific Dynamic Action 0 (unitless) included in above
Excretion : Respiration 0.17 ratio
Gametes : Biomass 0.18 ratio Walz, 1995, p. 445
Gamete Mortality 0.0001 1/d questionable
Mortality Coefficient 0.25 1/d Walz, 1995, p. 443
Exponential Mort. Coeff. 0.33 max/d Walz, 1995, p. 442
Carrying Capacity 2.5 mg/L LeCren & Lowe-McConnell, 1980, p. 260

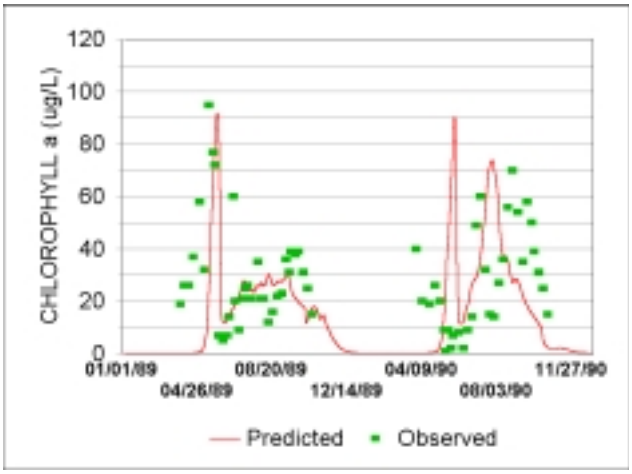

AQUATOX: Edit Animal
Load from Lib.
Save to Library
OK
Cancel
Print
Rotifer.
Gamete Mortality 0.0001 1/d questionable
Mortality Coefficient 0.25 1/d Walz, 1995, p. 443
Exponential Mort. Coeff. 0.33 max/d Walz, 1995, p. 442
Carrying Capacity 2.5 mg/L LeCren & Lowe-McConnell, 1980, p. 260
Trophic Interactions:
Preference: (ratio)
Egestion: (fraction)
References:
Sed. Refractory Detritus 0 0
Sed. Labile Detritus 0 0
Particulate Refrac. Detritus 0 0
Particulate Labile Detritus 0.4 0.15 Walz, 1995, p. 438
Diatoms 0.05 0.15 "
Blue-Greens 0.5 0.15 " cryptomonads
Greens 0.05 0.15 "
Macrophytes 0 0
Detritivorous Invertebrates 0 0
Herbivorous Invertebrates 0 0
Predatory Invertebrates 0 0
Forage Fish 0 0
Bottom Fish 0 0
Small Game Fish 0 0
Bioaccumulation Data:
Mean age or lifetime 4 days Walz, 1995, p. 442
Initial fraction that is Lipid (Wet Wt.) 0.03 prof. opinion
Mean weight 1.2E-7 g Walz, 1995, p. 441

In order to conduct "what if" exercises with the model, we will set the control options to remove point source loadings for nutrients and detritus (click on **Setup** then **Control Setup**). This effectively turns off the contributions of the metropolitan sewage treatment plant. (Another option would be to turn off the non-point source loadings.)

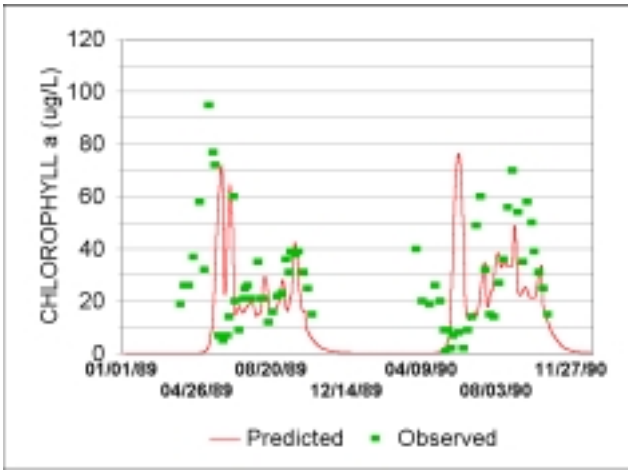


Using chlorophyll a as an indication of water quality, and plotting the **Export**ed results with observed values, we can see the normal predicted responses and those predicted if sewage effluent were diverted. As expected, diversion is predicted to result in lower chlorophyll and thus better water quality.

Standard prediction



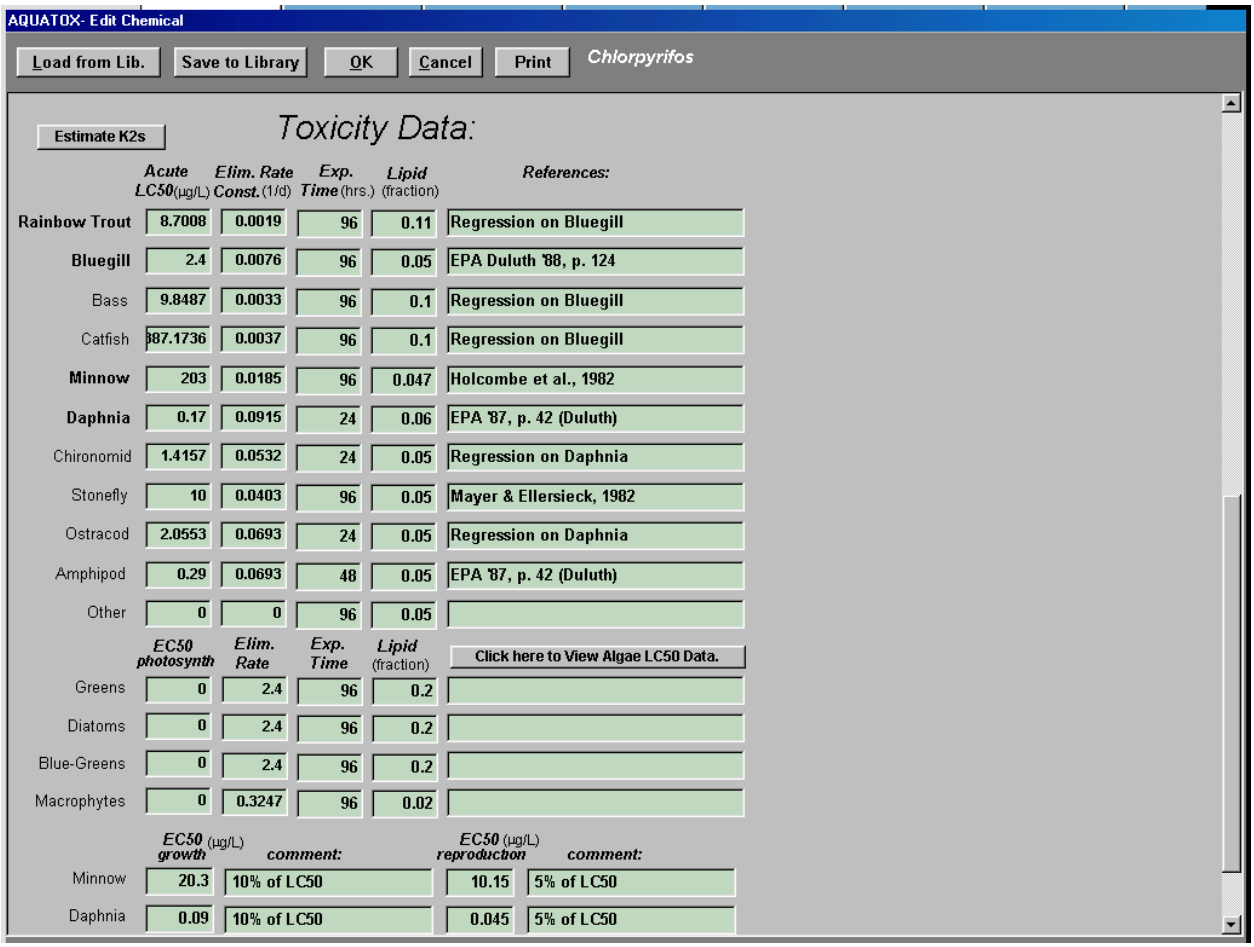
Prediction with sewage effluent diverted



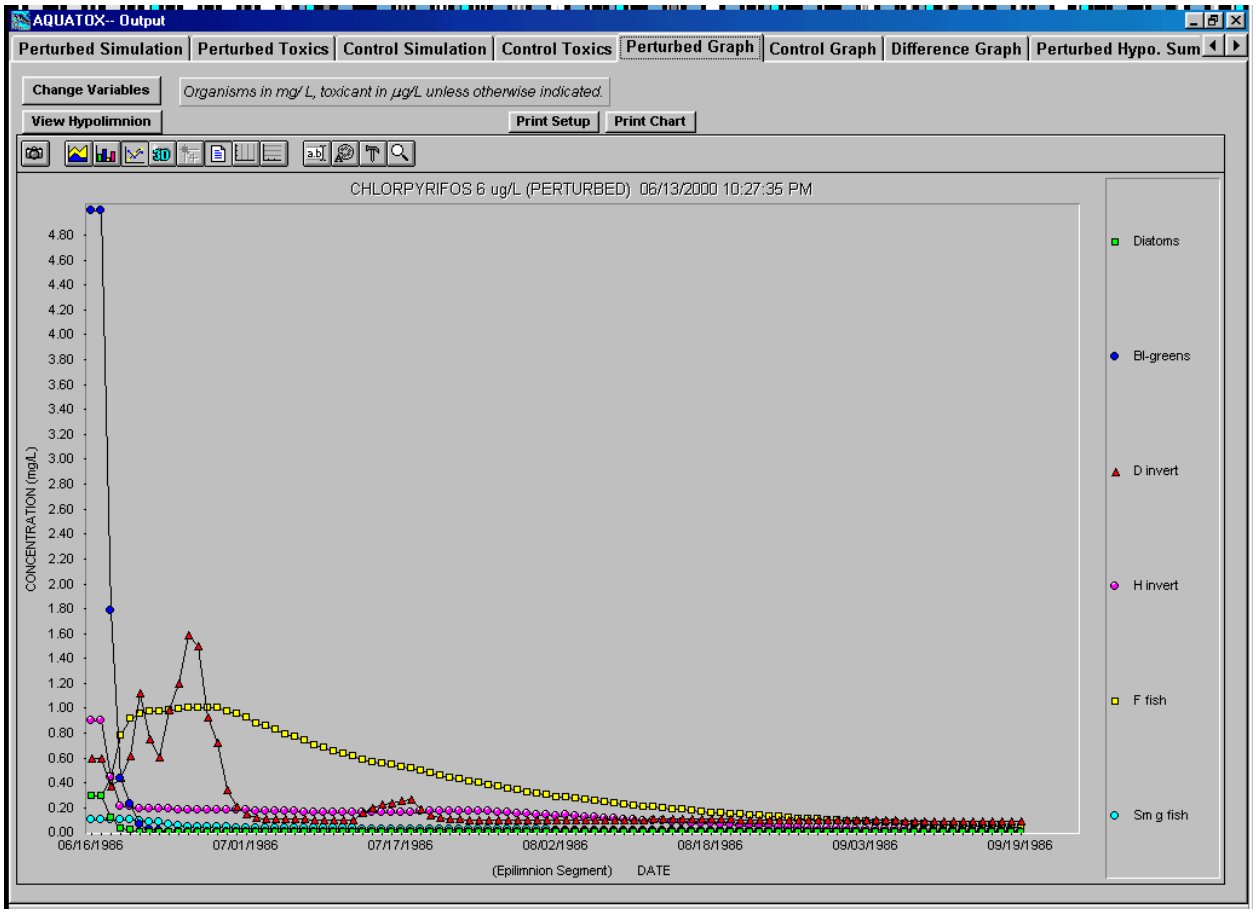
Other water quality parameters related to eutrophication and nutrients are also computed, such as dissolved oxygen, Secchi depth, nitrate, ammonia, and phosphate. The user could perform similar analyses with these parameters as was just shown with chlorophyll a. This would give a more complete picture of the lake's responses to proposed nutrient control scenarios, and whether water quality standards would be met. See **Volume 3: Model Validation Reports** document for a more detailed discussion of the application to this highly eutrophied lake.

3.2 Contamination by Organic Toxicants

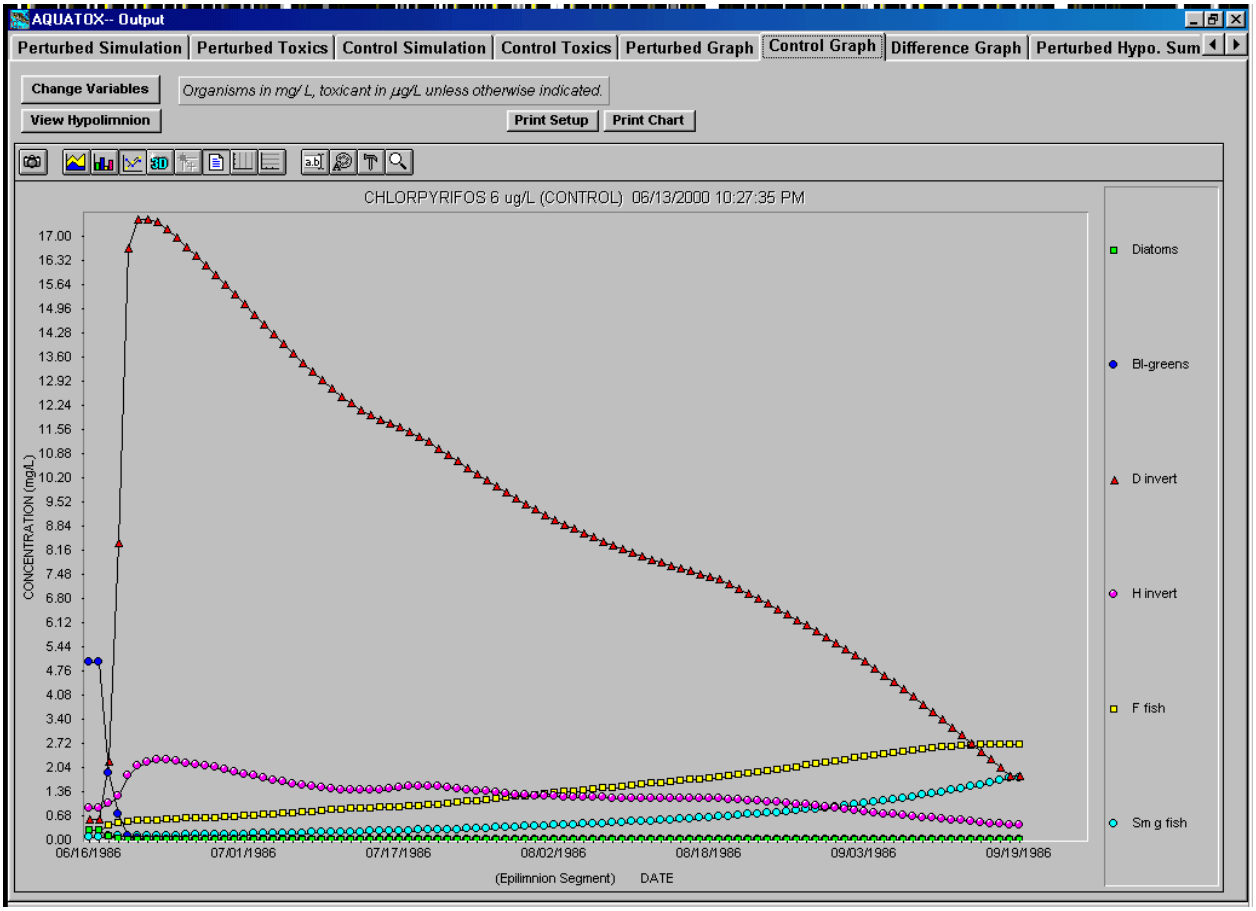
As the only general fate and effects model of potentially toxic chemicals in aquatic ecosystems, AQUATOX is well suited for risk assessment of organic toxicants. An earlier version was used in a comparative risk assessment of twenty-five pesticides. As an example, let's consider the ecological risk assessment of the pesticide chlorpyrifos in an experimental pond enclosure. Load the study *ChlorMed.aps* and click on **Chemical**. You will see the **Edit State Variable** window. First check to be sure that **Gas-phase conc**. is set to 0 and that the initial condition is 6.3 µg/L (we will start the simulation with an initial concentration and no loadings). Then click on **Edit Underlying Data** to get the chemical parameters. Click on **Toxicity Data** or page down to see the ecotoxicology parameters. The lipid fractions for the organisms should be as shown below. When they are correct, click on **Estimate K2s** (elimination rates) to be sure that estimates are up to date.(See **Volume 2: Technical Documentation** for a discussion of *K2*s.) Then save and go back to main menu to run the perturbed and control simulations. If you wish to evaluate biologic rates, that should be done in the **Setup** screen prior to running the simulations.



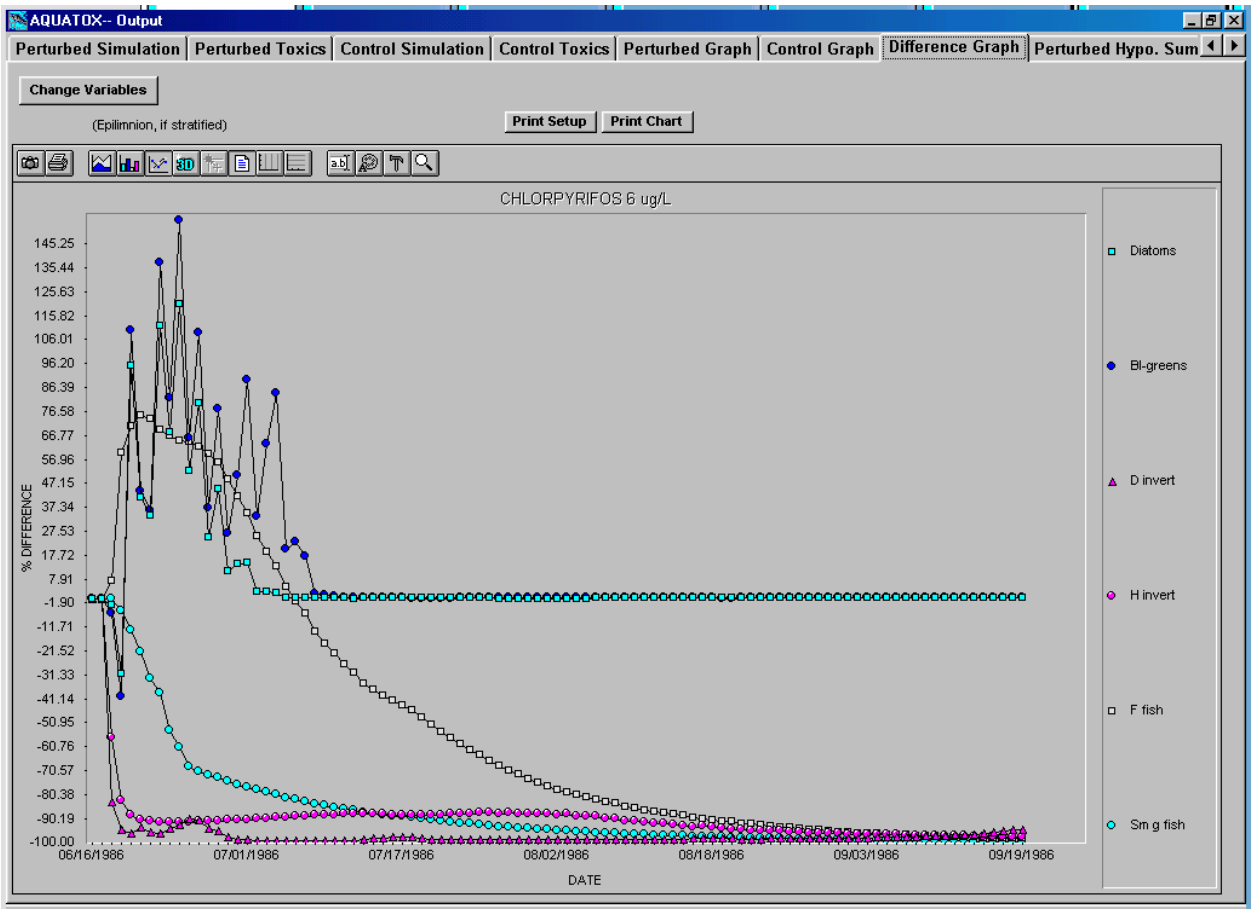
The impacts are substantial when contrasted with the Control simulation. In the perturbed graph the most obvious features are the immediate decline of most compartments with the exception of the forage fish (minnows).



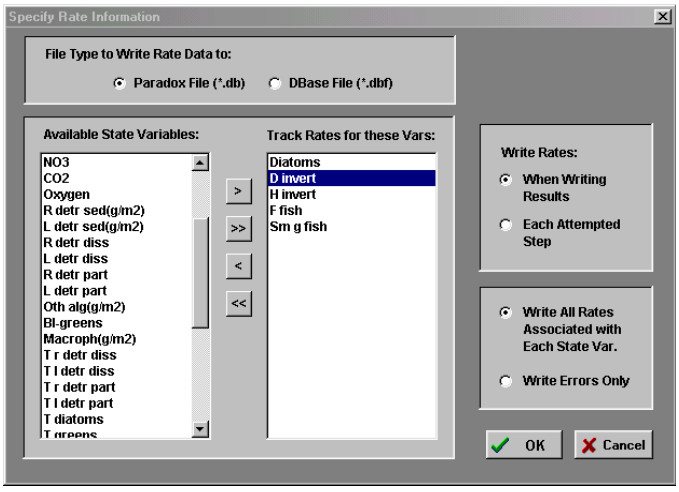
In the control plot we see a normal progression as first the zoobenthos, then the forage fish, then the small game fish become established in this experimental system.



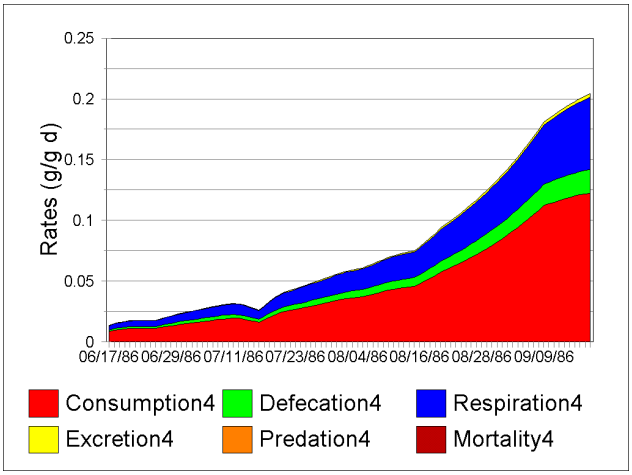
The difference graph shows the impact of the chlorpyrifos. It is obvious that a significant fraction of the invertebrates are killed immediately. However, the effects on fish are more subtle and interpretation of the output requires additional information.



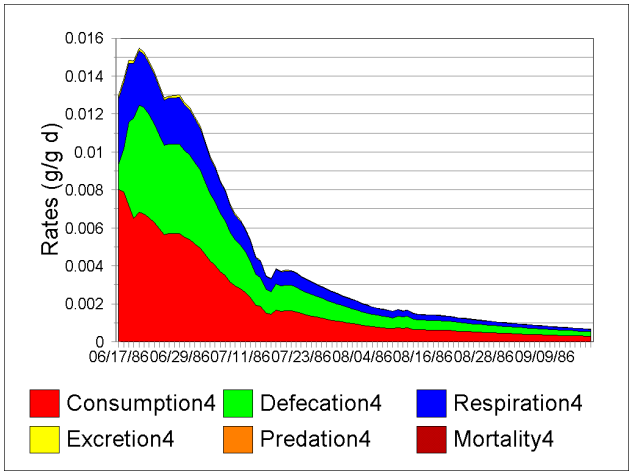
The rates were saved by choosing **Setup** from the main screen, **Save Biologic Rates**, and then **Rate Specifications**. The state variables and file type were chosen in the following screen. The plots were produced using Quattro Pro, but any spreadsheet or graphing program could be used.



Bluegill rates in control simulation

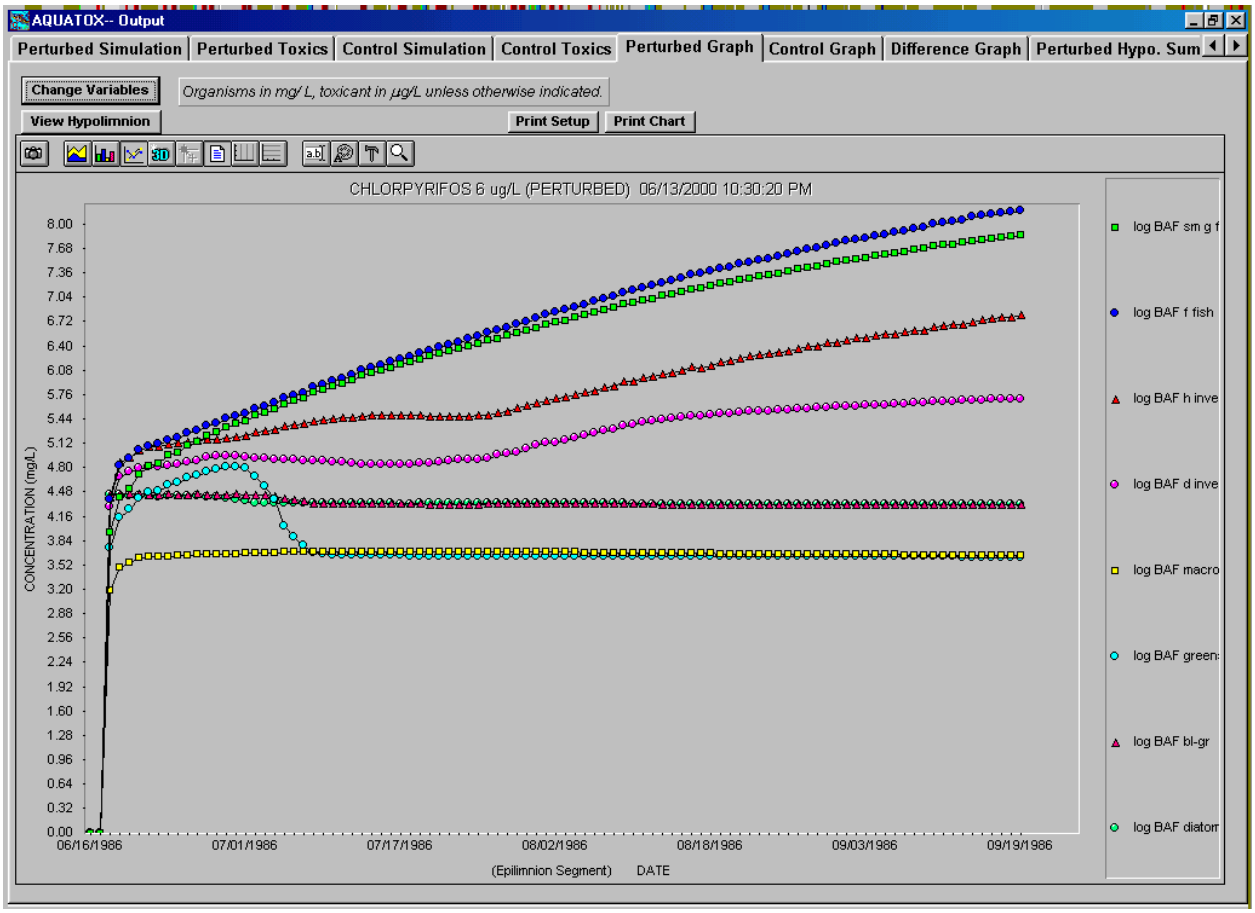


Bluegill rates with 6 µg/L chlorpyrifos initially



With chlorpyrifos, the small game fish (actually bluegill young-of-year) immediately suffer loss of food base; but, more important, the increase in defecation indicates chronic toxicity, which is paralleled by decreased consumption in the simulation. There is no acute toxicity as indicated by mortality, but the fish biomass declines steadily. Examination of the chemical record shows that bluegill have a laboratory LC50 of 2.4 µg/L The fact that bluegill are not killed can be explained by the rapid sorption of chlorpyrifos to sediments and therefore decreased bioavailability.

Chlorpyrifos is a bioaccumulative chemical. A plot of bioaccumulation factors indicates that there is biomagnification up the food-chain and that steady-state has not been achieved for the fish in the three-month simulation.

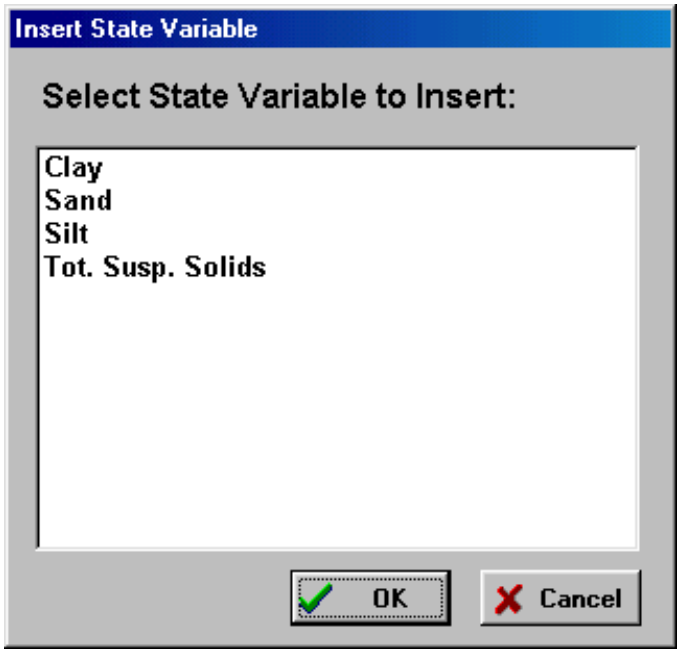


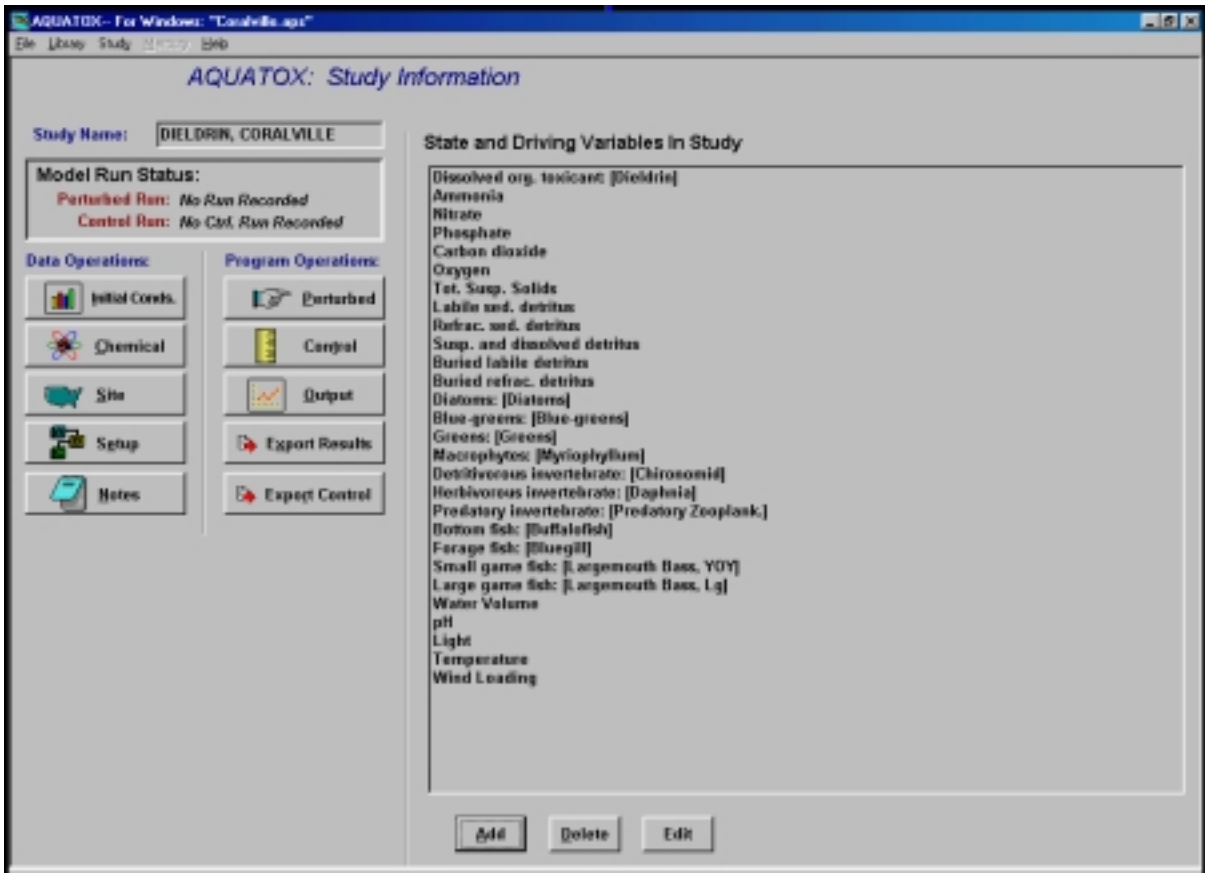
3.3 Multiple Stressors Due To Agricultural Runoff

In our example, we will model a run-of-the-river reservoir receiving extensive agricultural runoff and minimal municipal and industrial effluents (Park, 1999a). In the 1970s approximately 90% of the watershed of Coralville Reservoir, Iowa, was in agricultural land (MacDonald and MacDonald, 1976). Water quality was so poor that the lake was referred to locally as the "Dead Sea." We will use the reservoir study ***Coralville.aps*** as a starting point. Open the file, then click on **File** and **Save As**, and name it ***AgricRes.aps*** so we don't write over the default reservoir study by mistake. Also, change the Study Name to "CORALVILLE RESERVOIR" (this will be the heading for the graphs).

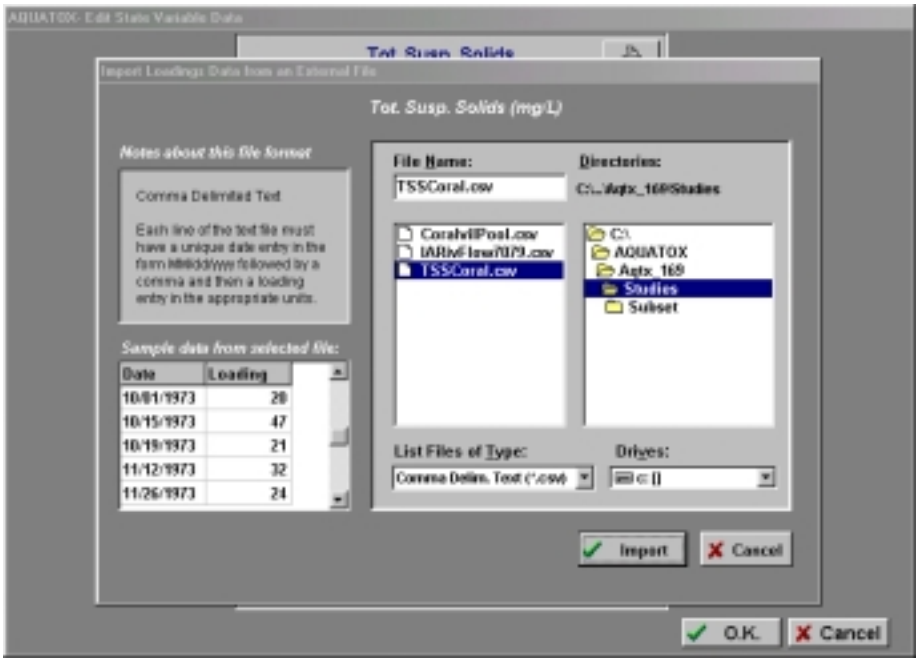
Controlling Nutrients and Sediments—Because this reservoir receives a large quantity of suspended sediments, we need to load observed total suspended solids (TSS). Clay, silt, and sand are only available if the site is a stream. Suspended algae and detritus are subtracted from the observed TSS and the difference is considered to be suspended inorganic sediments. These are used in calculating the extinction coefficient and the Secchi depth.

Click on **Add** at the bottom of the state variable list and choose **Tot. Susp. Solids**. In the main screen we then see this as an additional state variable.





Double-click on **Tot. Susp. Solids** obtain the loadings screen. Then click on **Use Dynamic Valuation** and **Import** to load the file ***TSSCoral.csv***.

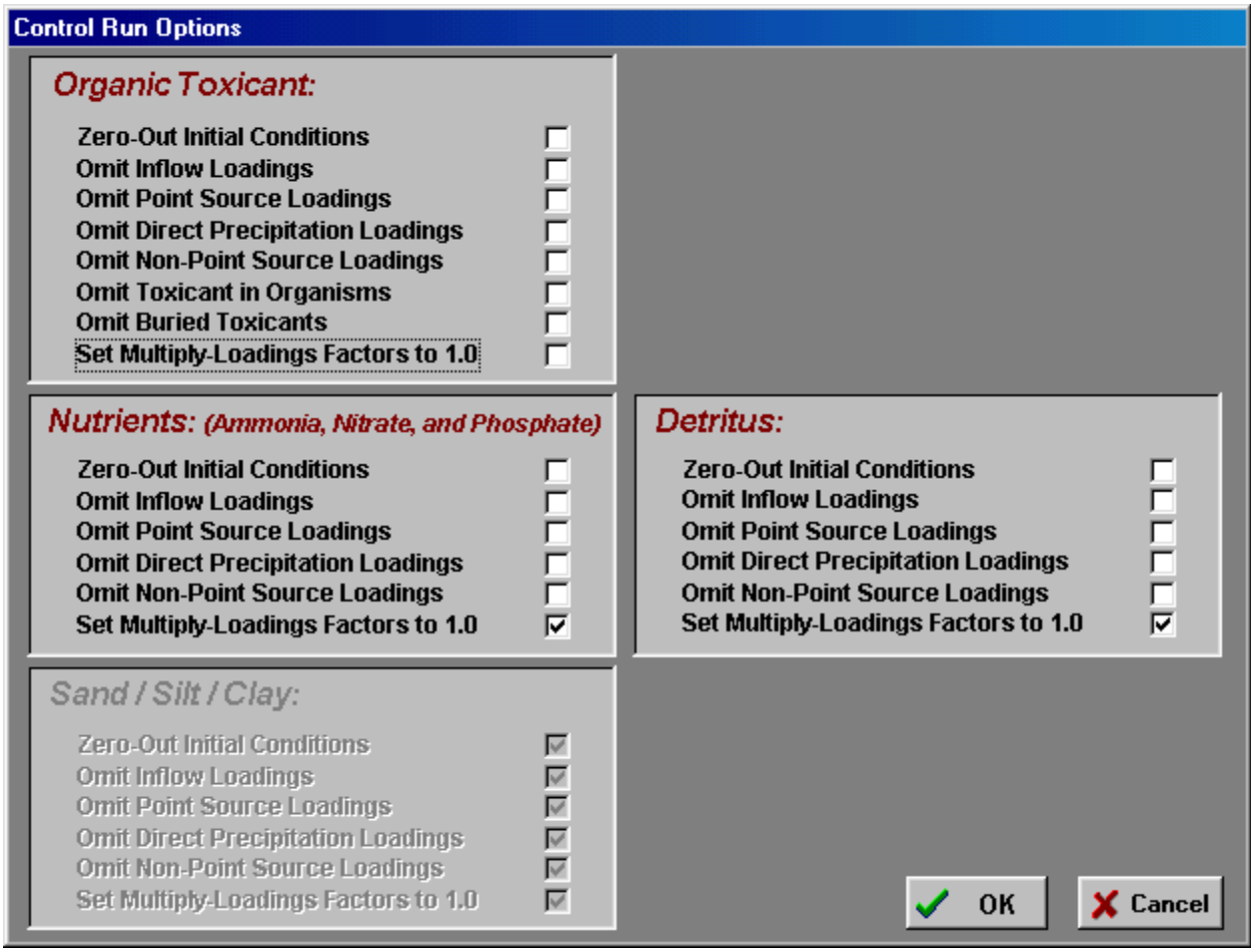


Click on **Initial Conditions** to see the initial values for all the state variables. Dieldrin is 0 because we will let the model compute the concentration in the reservoir.

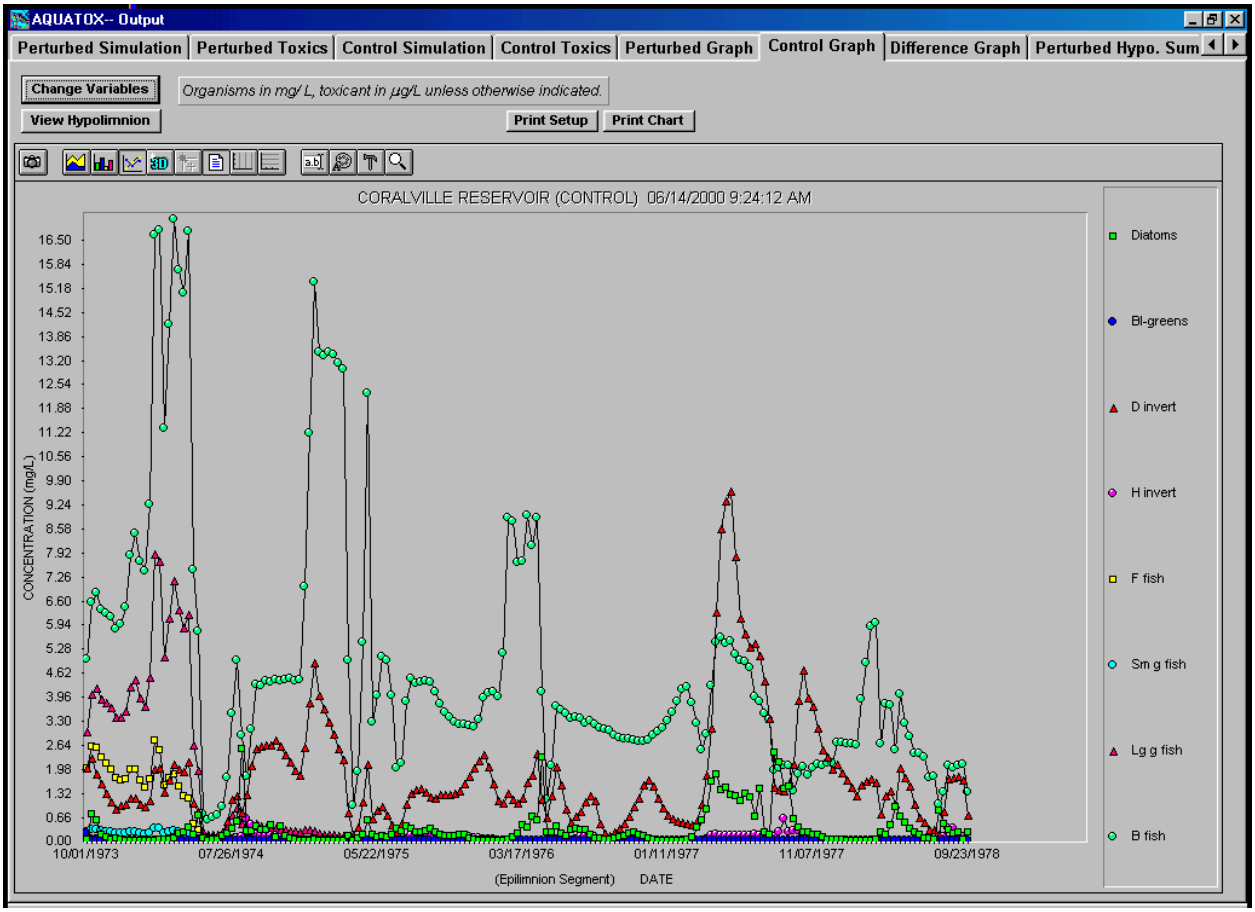
State Variable Name	Init. Cond.	Units	Org. Tox. I.C.	Tox. Units
Dissolved org. toxicant: [Dieldrin]	0	ug/L		
Ammonia	0.08	mg/L		
Nitrate	4.9	mg/L		
Phosphate	0.21	mg/L		
Carbon dioxide	12	mg/L		
Oxygen	6.5	mg/L		
Tot. Susp. Solids	20	mg/L		
Labile sed. detritus	2.5	g/sq.m	0	ug/kg
Refrac. sed. detritus	5	g/sq.m	0	ug/kg
L detr diss	0.5994	mg/L	0	ug/kg
R detr diss	0.0666	mg/L	0	ug/kg
L detr part	0.0666	mg/L	0	ug/kg
R detr part	0.0074	mg/L	0	ug/kg
Buried labile detritus	2	Kg/cu.m		
Buried refrac. detritus	2	Kg/cu.m		
Diatoms: [Diatoms]	0.05	mg/L	0	ug/kg
Blue-greens: [Blue-greens]	0.21	mg/L	0	ug/kg
Greens: [Greens]	0.05	mg/L	0	ug/kg
Macrophytes: [Myriophyllum]	0.1	mg/L	0	ug/kg
Detritivorous invertebrate: [Chironomid]	2	mg/L	0	ug/kg
Herbivorous invertebrate: [Daphnia]	0.023	mg/L	0	ug/kg
Predatory invertebrate: [Predatory Zoopl	0.1	mg/L	0	ug/kg
Bottom fish: [Buffalofish]	5	mg/L	1200	ug/kg
Forage fish: [Bluegill]	2	mg/L	0	ug/kg
Small game fish: [Largemouth Bass, YOY]	0.238	mg/L	0	ug/kg
Large game fish: [Largemouth Bass, Lg]	3	mg/L	0	ug/kg

Click on **Setup** and make sure that the simulation dates correspond to, or are less than, the range of dates for TSS, 10/1/1973 to 9/30/1978. Be careful, if you enter "10/1/73" it will be interpreted as "10/01/2073." Because observed TSS values are being used in lieu of dynamically simulated inorganic sediments, the capability of the model to repeat a time-series loading should not be used for TSS unless all other loadings, particularly inflow, are restricted to the same range. Otherwise, the model will extrapolate the TSS beyond the observed dates and obtain unacceptable estimates of suspended sediments. Note that the 5-year simulation may be quite lengthy on a slow machine; you may wish to decrease the period.

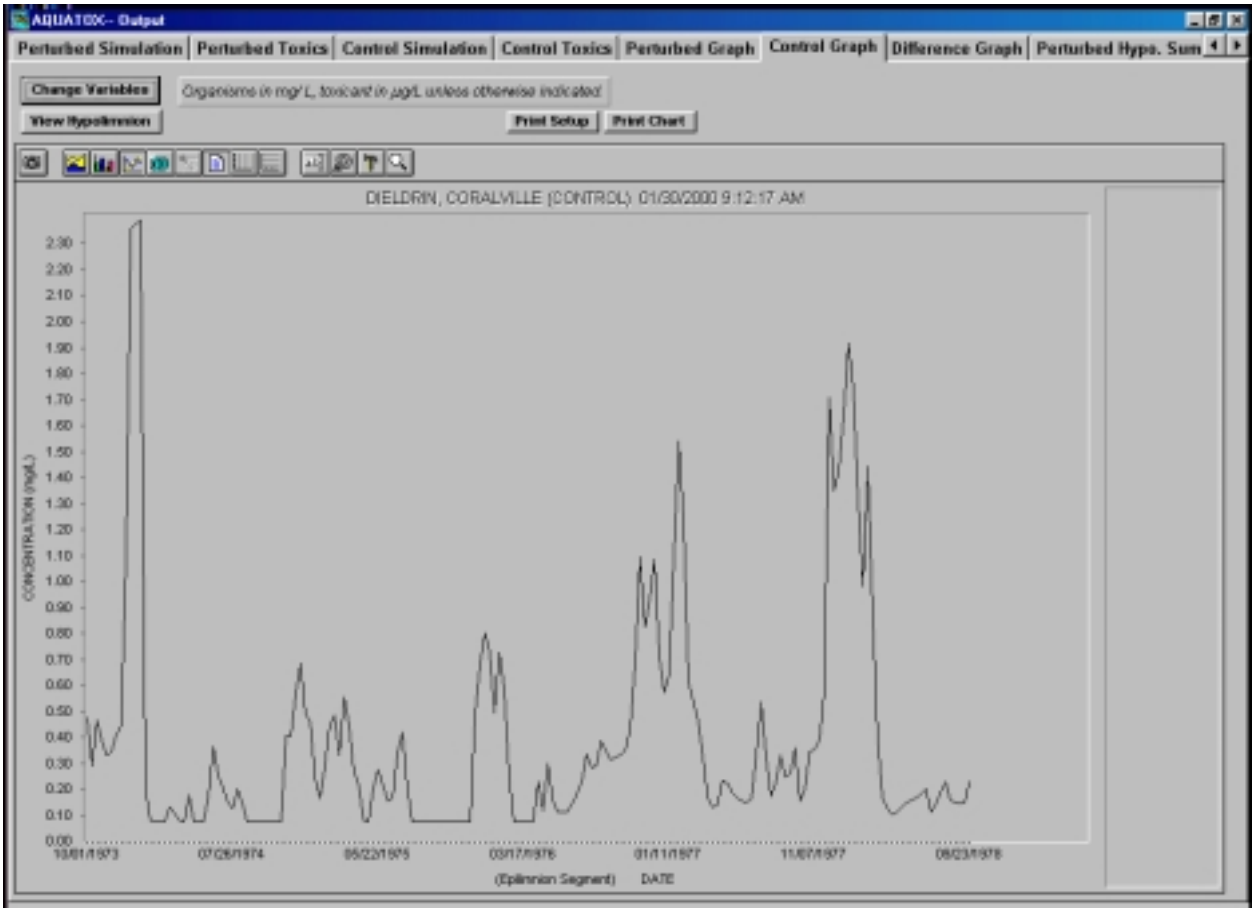
First we will investigate the impact of nutrient reduction, most likely through best management practices, without any change in loadings of dieldrin or inorganic sediments. Click on **Control Setup** and uncheck all the **Organic Toxicant** controls, and check **Set Multiply Loadings Factors to 1.0** for **Nutrients** and **Detritus**. Then, going back to the main screen, double-click on ammonia, nitrate, phosphate, and suspended and dissolved detritus and enter a multiplicative loading of 0.5, if not already done, on the **Edit State Variable Data** screen for each. In doing so, we have set the model so that nutrients and detritus will be halved in the perturbed run and kept unchanged for the control run. Dieldrin will be present in both simulations. This demonstrates the power of the control settings to set up various pollution control scenarios.



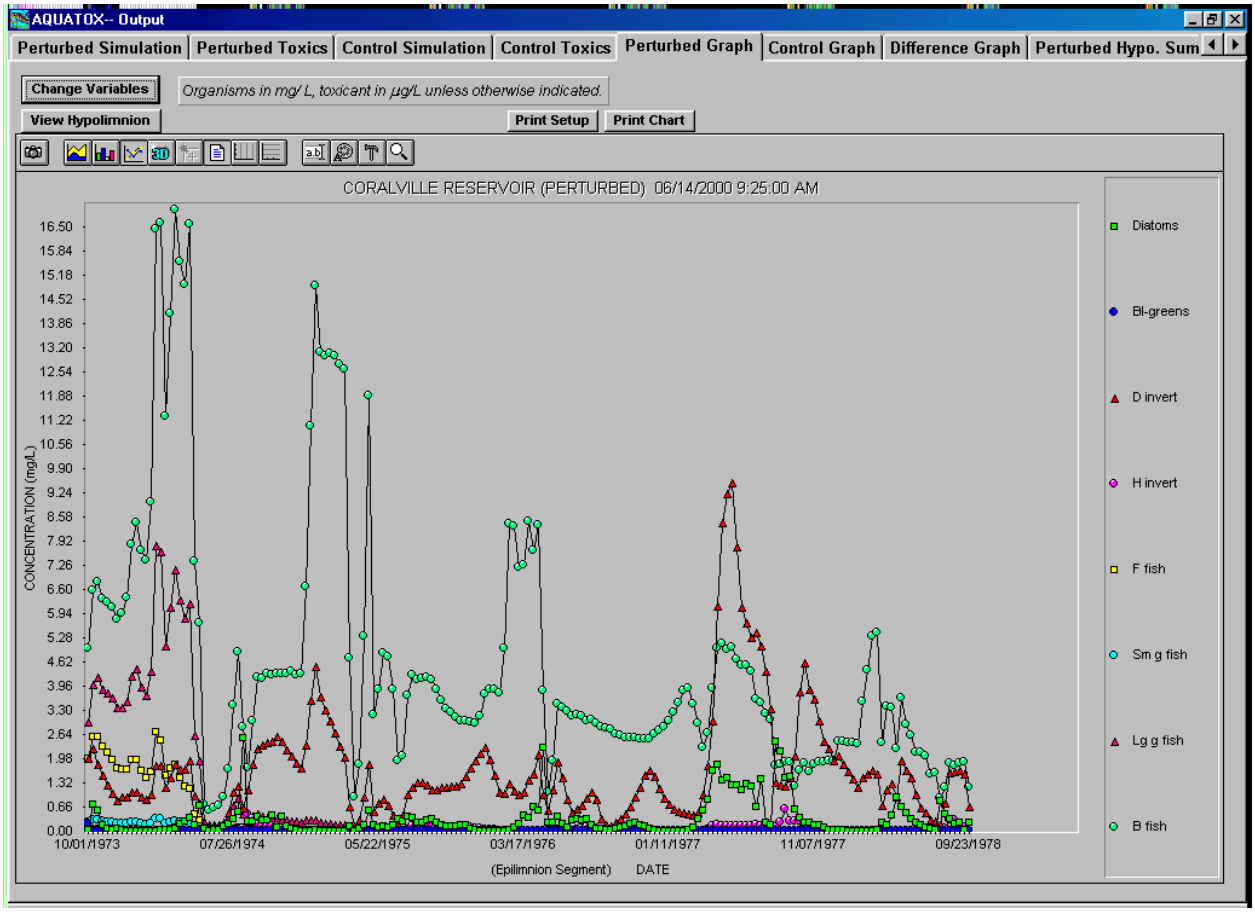
Run the simulation without any additional changes, clicking on **Perturbed** and **Control**. Select **Output,** and view the **Control** graph. Note that detritivorous invertebrates have a high biomass, reflecting the large influx of detritus from upstream. Diatom blooms occur periodically, with maximum biomass of about 16 mg/L during drought conditions in 1977.



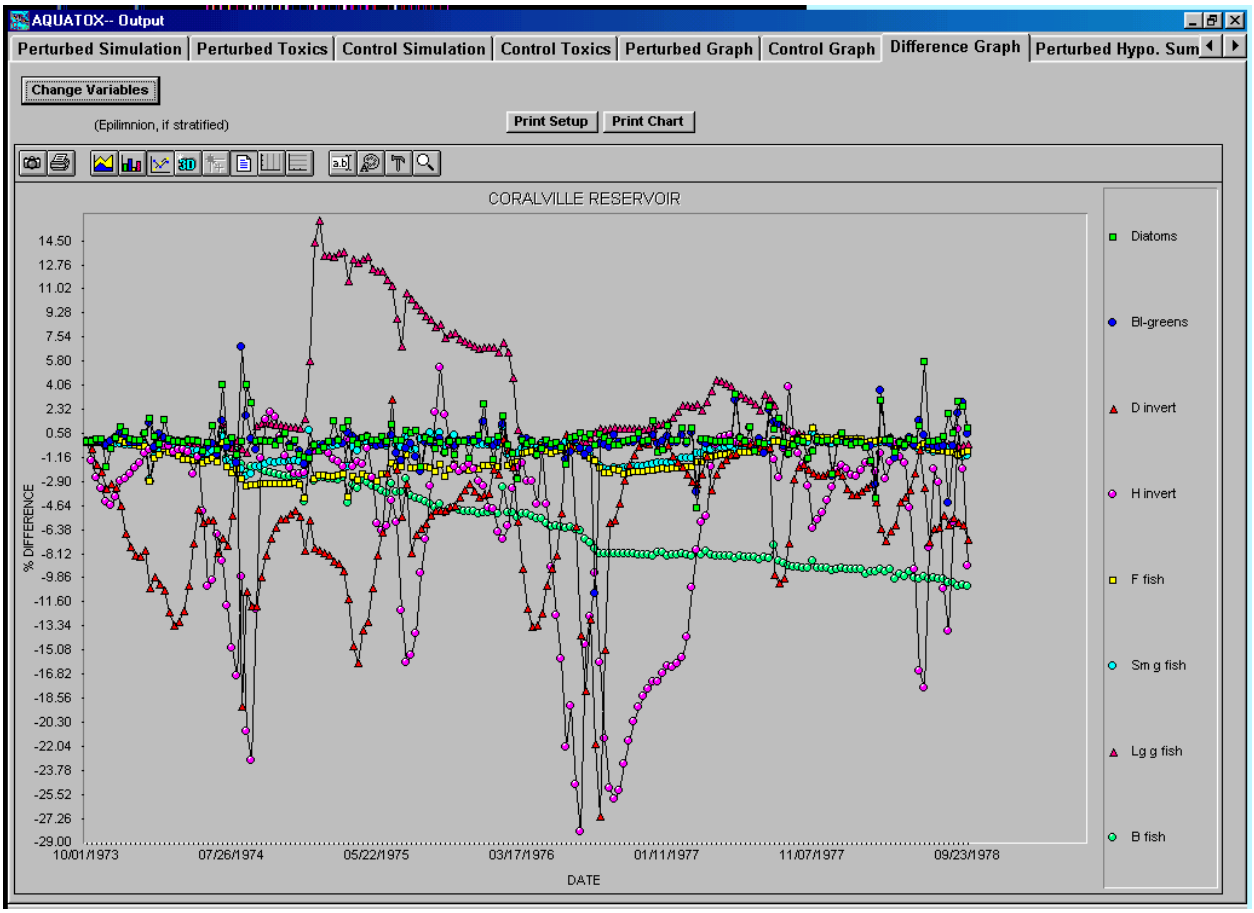
If we plot Secchi depth we find that the minimum is 8 cm, with a maximum of about 2.5 m and a mean of less than 1 m. Note that if you plot only one variable the graphing routine plots it in black, and no legend appears. Also note that the label on the vertical axis reads "Concentration"; you may wish to edit this.

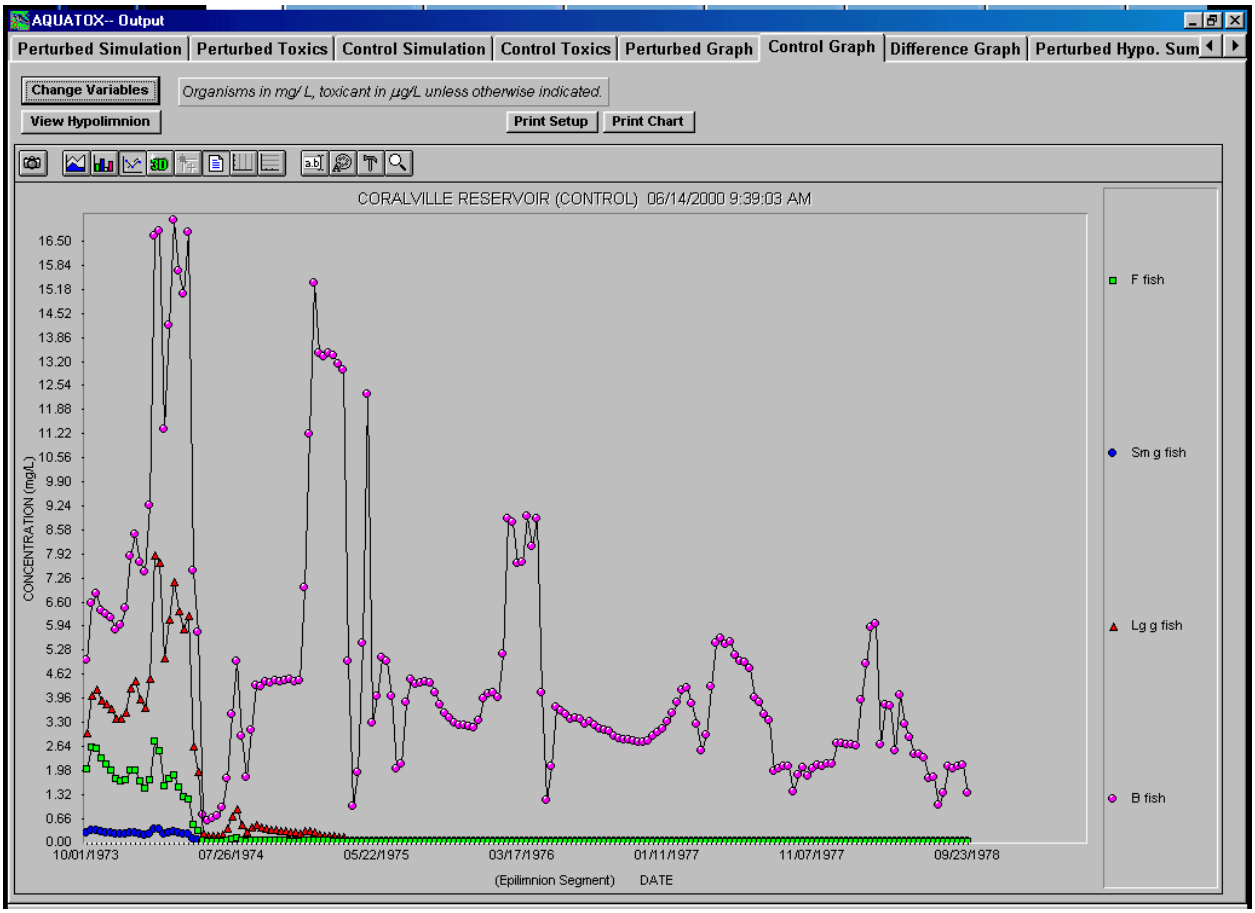


Now view the **Perturbed** graph. The similarity with the Control graph suggests that few changes would occur in water quality if the nutrient and detritus loads are reduced by one-half. The diatom blooms are virtually unchanged. The most obvious change is a small decline in forage fish (blue-gills), which is probably linked to a corresponding decline in detritivore biomass.

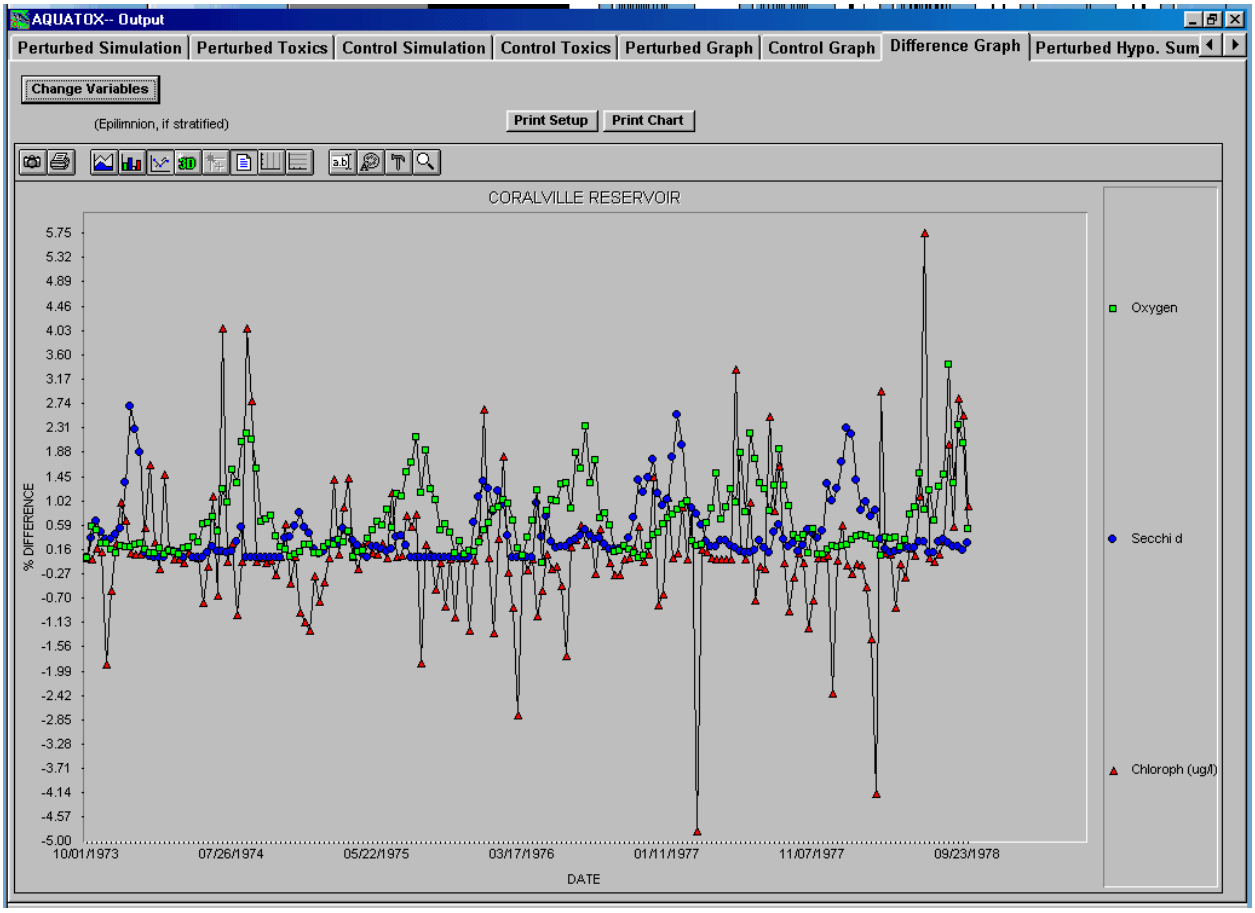


A better way to portray the changes is by plotting a **Difference** graph. Because we have set the nutrient and organic loadings in the perturbed simulation to half the normal values, a positive percent difference means an increase in biomass with decreasing nutrient and organic loadings. (Remember that the **Difference** graph plots the percent difference of **Perturbed** minus **Control.**) We also will plot bottom fish (buffalofish), which were so abundant in Coralville Reservoir that they supported a commercial fishery in the early 1970s. Based on this graph and examination of predicted rates for the invertebrates and fish, which were saved and plotted in Quattro Pro, we observe that invertebrate detritivores declined slightly due to decreased detritus loadings; this caused a decline in blue-gills, followed by declines in their predators, bass. Eventually, in the absence of competition, buffalofish are predicted to increase. Caution should be exercised in interpreting difference graphs; these are plotted as percent changes, and small absolute differences are magnified. For example, due to the toxicity of dieldrin, bass exhibit very low biomass values, even in the control. This can be seen by plotting just the fish in the control simulation.



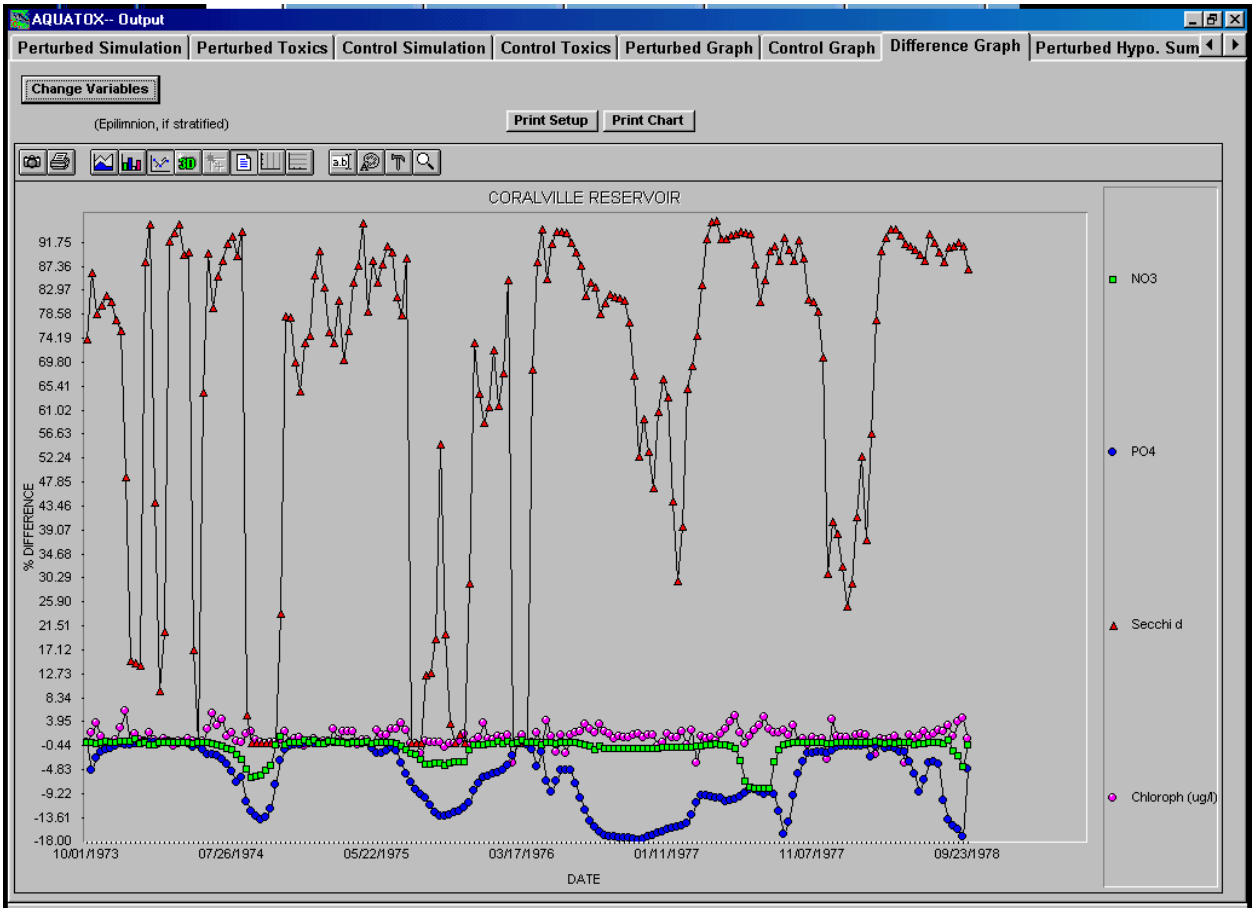

AQUATOX-- Output
Perturbed Simulation
Perturbed Toxics
Control Simulation
Control Toxics
Perturbed Graph
Control Graph
Difference Graph
Perturbed Hypo. Sum
Change Variables
Organisms in mg/ L, toxicant in µg/L unless otherwise indicated.
View Hypolimnion
Print Setup
Print Chart
CORALVILLE RESERVOIR (CONTROL) 06/14/2000 9:39:03 AM
CONCENTRATION (mg/L)
16.50
15.84
15.18
14.52
13.86
13.20
12.54
11.88
11.22
10.56
9.90
9.24
8.58
7.92
7.26
6.60
5.94
5.28
4.62
3.96
3.30
2.64
1.98
1.32
0.66
0.00
10/01/1973
07/26/1974
05/22/1975
03/17/1976
01/11/1977
11/07/1977
09/23/1978
(Epilimnion Segment) DATE
F fish
Sm g fish
Lg g fish
B fish

If we plot the difference graph for the key environmental indicators, oxygen, Secchi depth, and chlorophyll, we see that halving the nutrient and detrital loadings improves the water quality only slightly as indicated by slightly decreased chlorophyll levels and slightly increased Secchi depths.

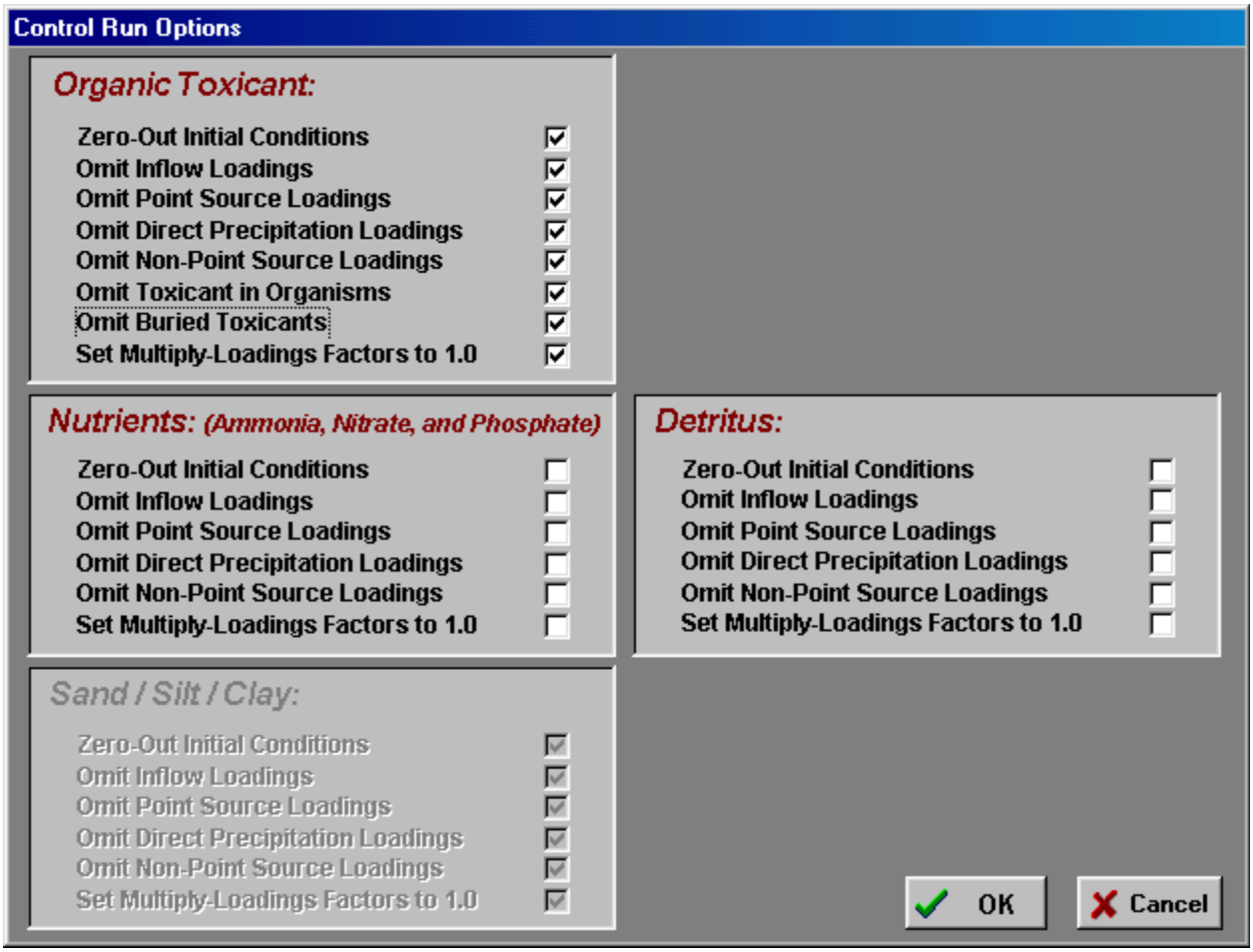


Having seen the effects of halving the nutrient and detritus loadings, let us now investigate the effects of suspended sediments. In this run-of-the-river reservoir most of the suspended solids are silt and clay, and most are from upstream. In the unlikely event that best management practices were to halve the TSS without altering the other pollutants, what would be the impacts on the Coralville ecosystem? This is easily analyzed with AQUATOX. Close the **Output** window, open the **Setup** window, and choose **Control Setup**. Now uncheck the **Nutrient** and **Detritus** choices. In the main window double-click on each of the nutrients and suspended detritus and set the multipliers back to 1.0; then double-click on **Tot. Susp. Solids** and set the **Multiply loading** to 0.5. Then click **Perturbed** (but do not run **Control**) to obtain a run that is perturbed only in that TSS is one-half that in the control.

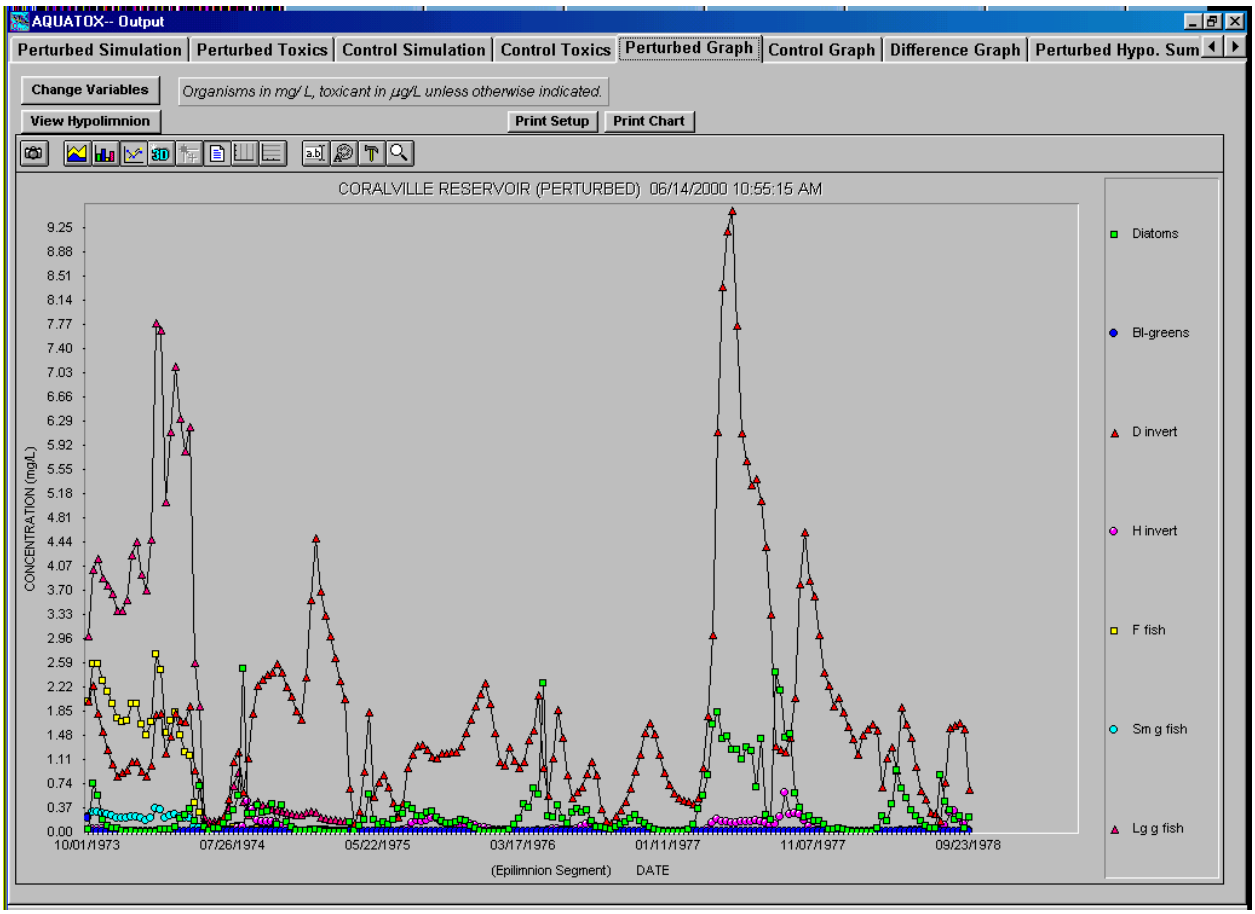
Click **Output** and plot Secchi depth, chlorophyll a, phosphate, and nitrate in the **Difference** graph. By decreasing TSS, and hence inorganic sediments, turbidity decreases, and phytoplankton are not as severely light limited in the simulation. In turn, phosphate decreases—almost certainly becoming limiting for the phytoplankton. Chlorophyll a does not increase significantly, probably because of grazing pressure by invertebrates.



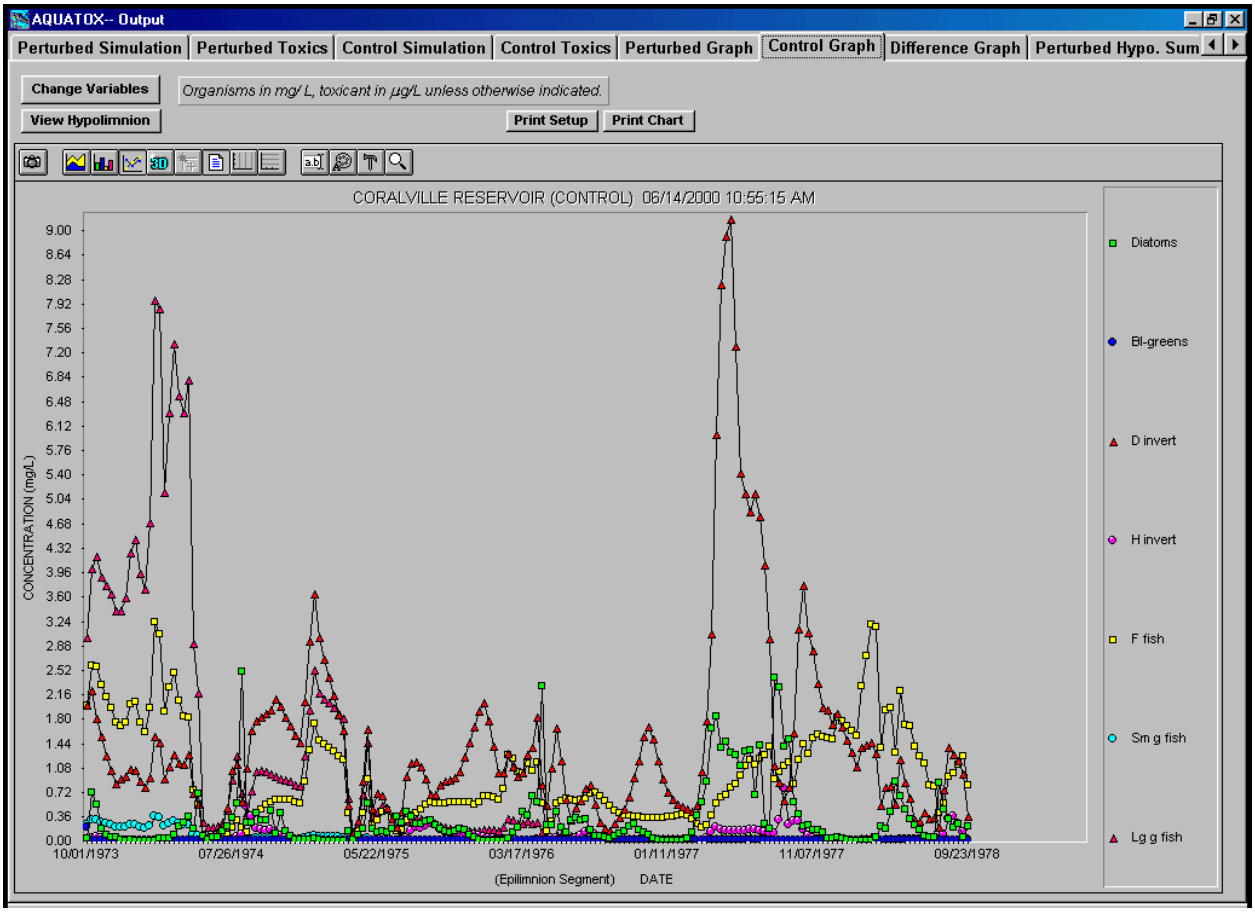
Controlling Pesticides—Next we will examine the effects of the dieldrin independent of the nutrients, detritus, and TSS. Similar to the example of esfenvalerate in the pond, we will use the perturbed run to simulate the toxicant and the control run without the toxicant. Therefore, close the **Output** window, then set the multiplicative loading for TSS back to 1.0, open the **Setup** window, and choose **Control Setup**. Now set the remaining options back to their original state, with all the **Organic Toxicant** choices checked, and the **Nutrient** and **Detritus** choices unchecked.



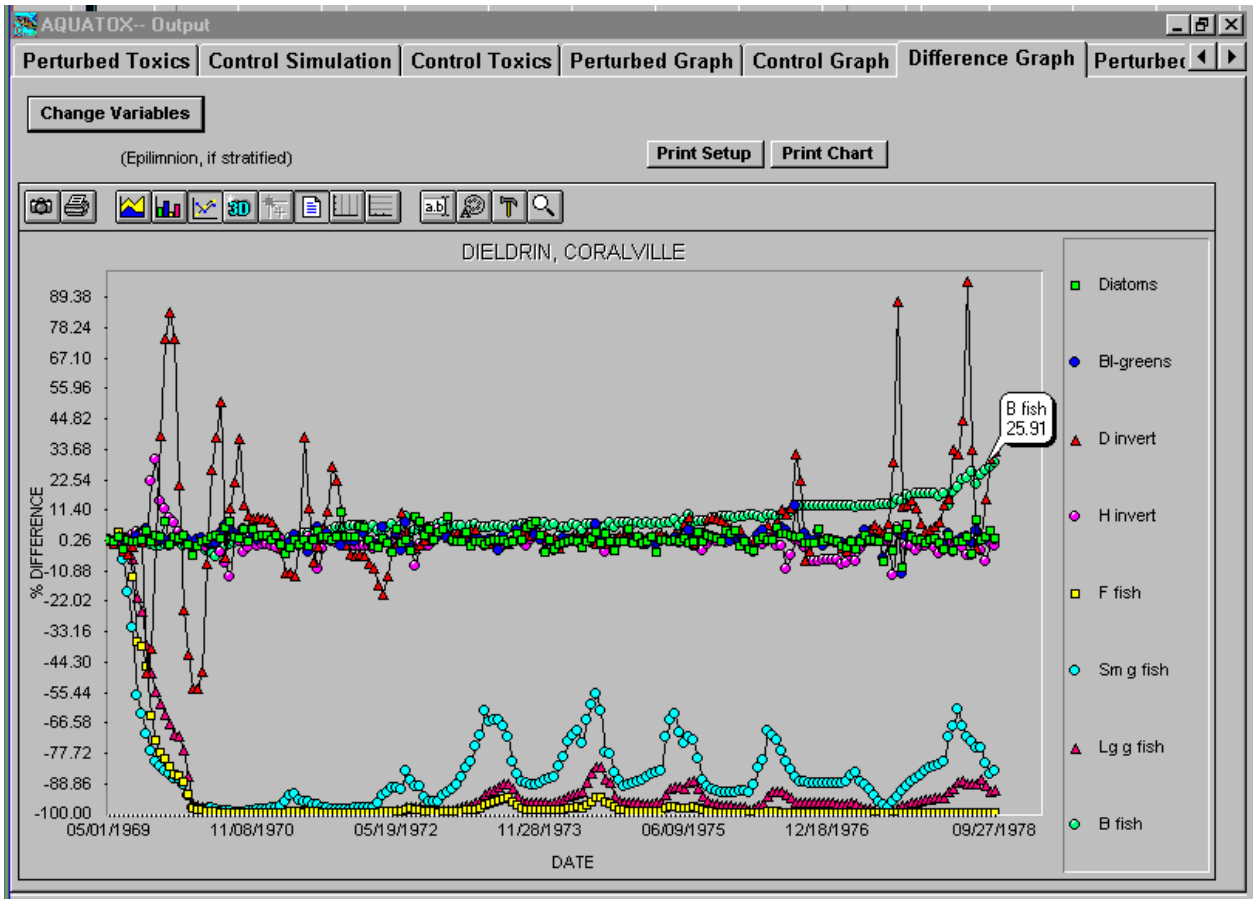
Click **Perturbed** and **Control** to re-run the simulations. The perturbed graph shows the effects of dieldrin on the default state variables. You can plot other variables by clicking on **Change Variables**.



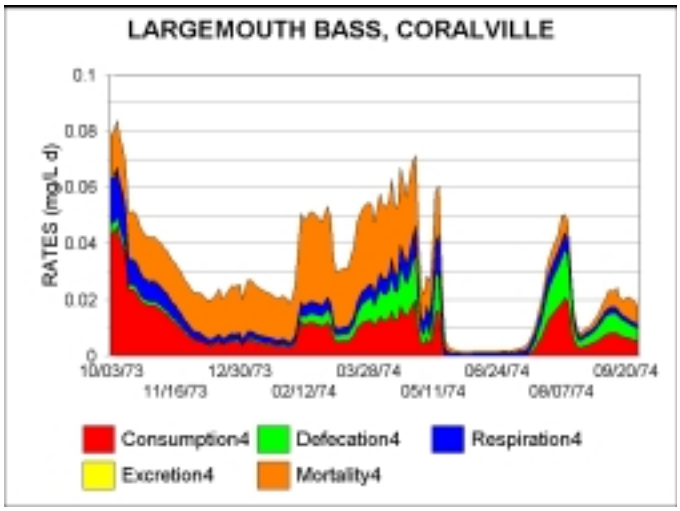
The control graph shows the seasonal patterns in biomass without dieldrin. Note that forage fish (bluegill) are relatively important throughout the simulation, in contrast to the pattern shown in the perturbed graph.



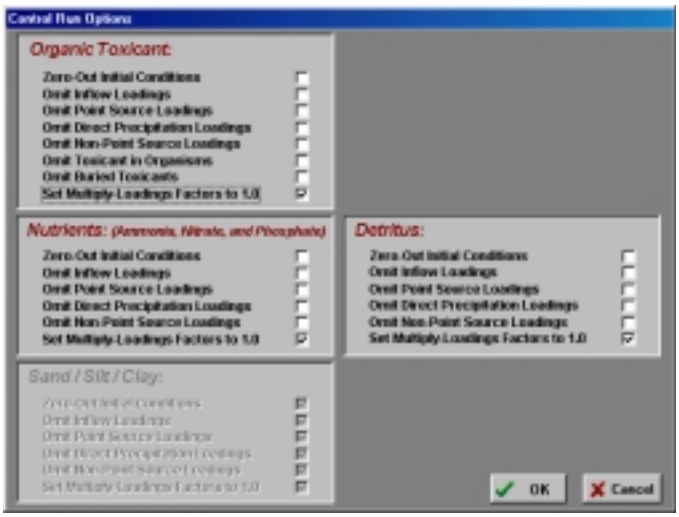
The differences between the perturbed and control graphs are emphasized in the difference graph. The difference is obtained by subtracting the control biomass from the perturbed biomass, so negative values indicate relatively low biomass values in the perturbed simulation (in other words, in the presence of dieldrin). The decline of all fish except the hardy buffalofish is easily seen. The chironomids (invertebrate detritivores) benefit from the decreased predation and exhibit positive values.

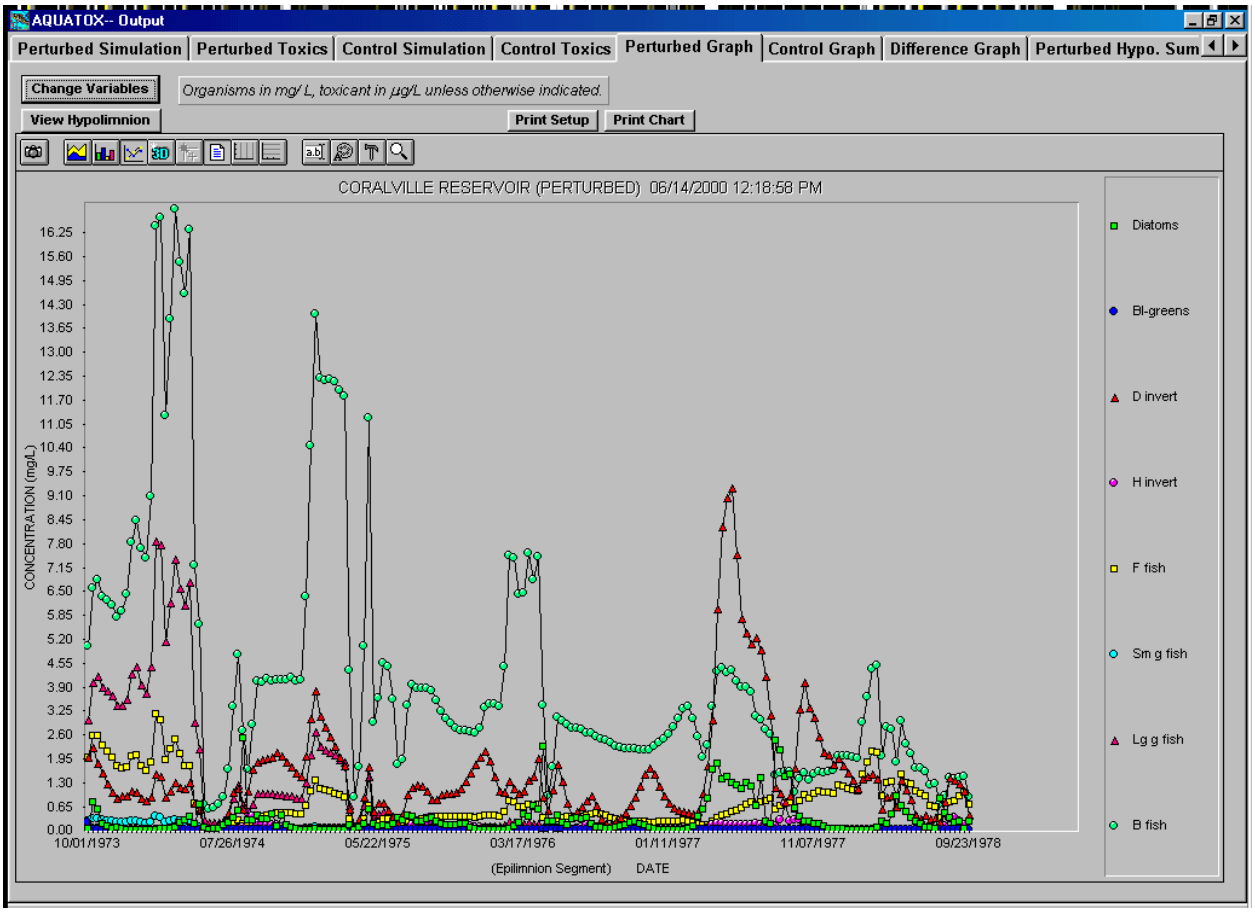


From these results, we postulate that the decline in fish is a combination of direct and indirect effects of dieldrin. We can examine the rates for largemouth bass by clicking on **Setup** in the main screen and **Save Biologic Rates** and **Rate Specifications**, then choosing **Lg g fish** prior to running the model. The rates will be saved, with Paradox format as the default, in the Output subdirectory. The rates can be plotted in a spreadsheet program. In this example, consumption declines due to chronic toxicity and loss of bluegill forage base, and mortality increases in part due to acute toxicity. Defecation increases due to the modeled effect of chronic toxicity on assimilation. This illustrates the use of biologic rates for analyzing cause and effect relationships.

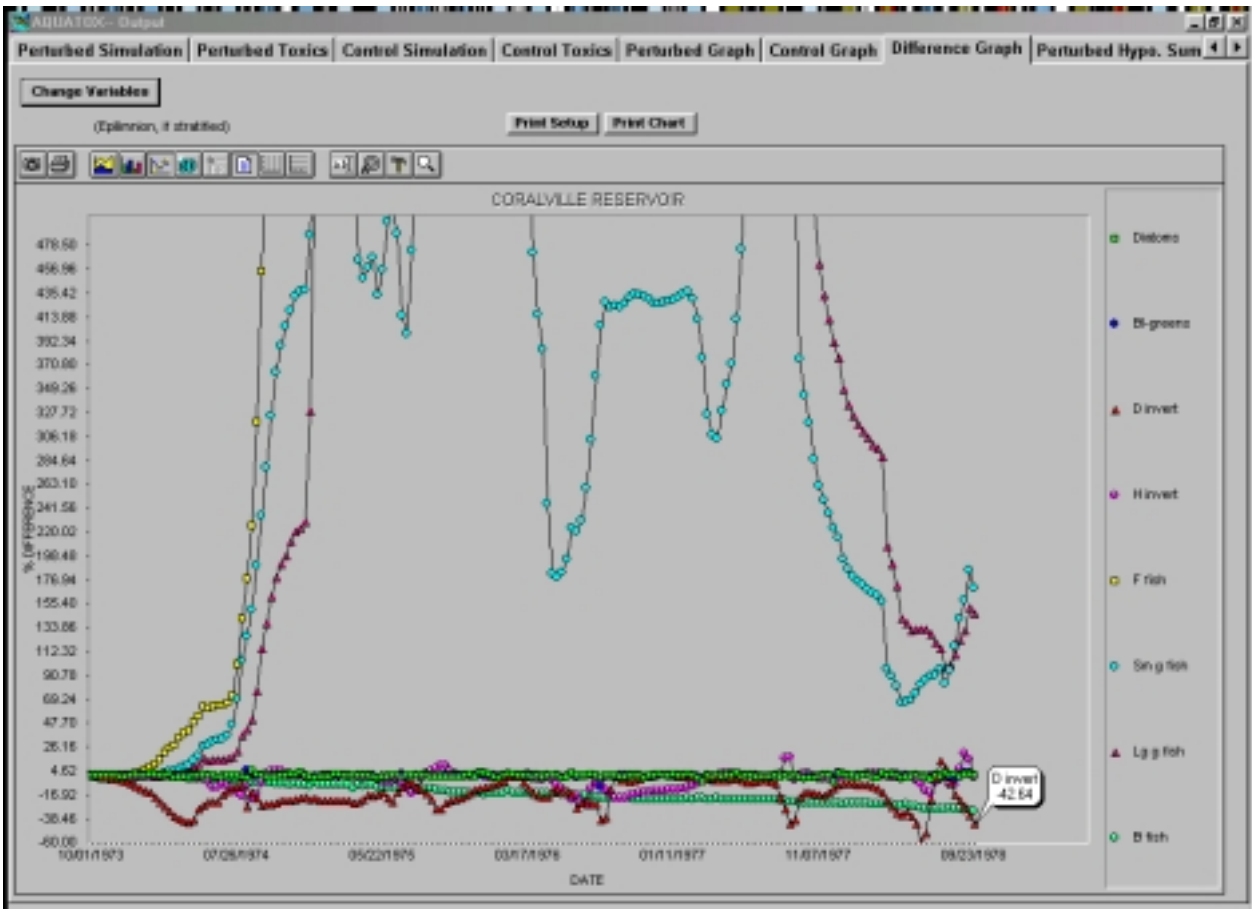


Controlling All Pollutants—Finally, we can examine the effects of decreasing all pollutants from agricultural runoff simultaneously in the perturbed simulation. Dieldrin was set to zero and the nutrient and organic matter multiplicative loading factors were set to one-half. As we have seen from the above applications, there are many complex interactions, and comparing the perturbed and control graphs is difficult.

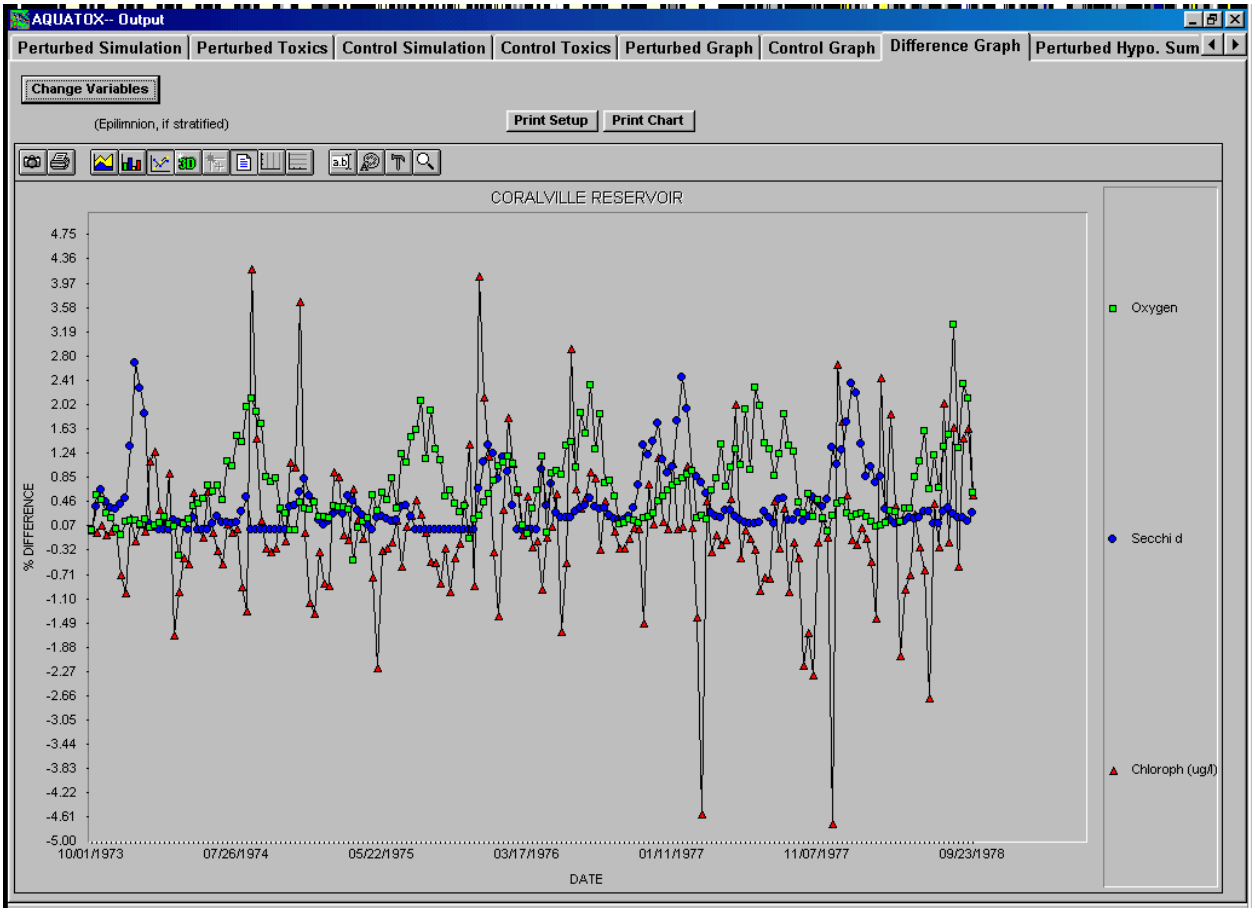




However, the difference graph provides a direct comparison. Bluegill and bass increase significantly in the absence of dieldrin. Chironomids decline due to increased predation pressure. The buffalofish exhibit a long-term decline due to loss of chironomid forage because of increased competition. Algae, herbivorous zooplankton, and labile detrital sediments (not shown) are relatively unchanged.



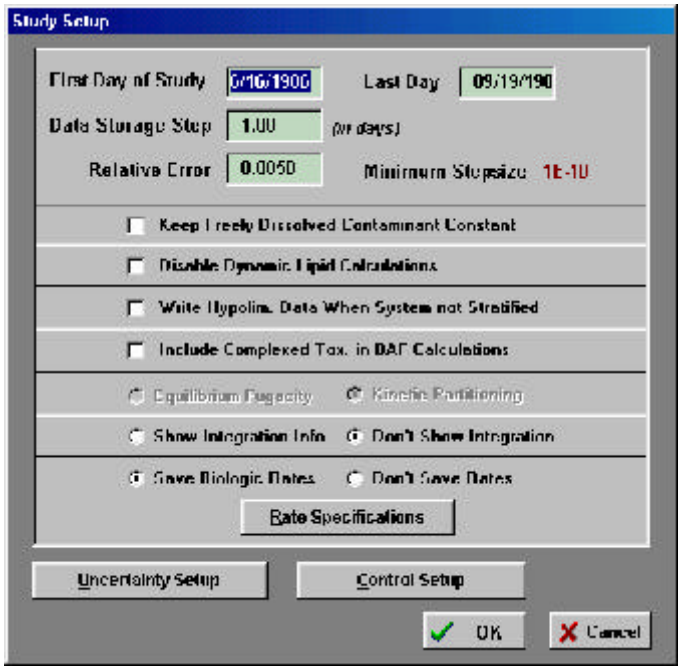
To better determine the effects on water quality, we will plot several environmental indices in a difference graph. We see that chlorophyll a is generally slightly lower with nutrients halved, oxygen is slightly increased, and Secchi depth is slightly improved.



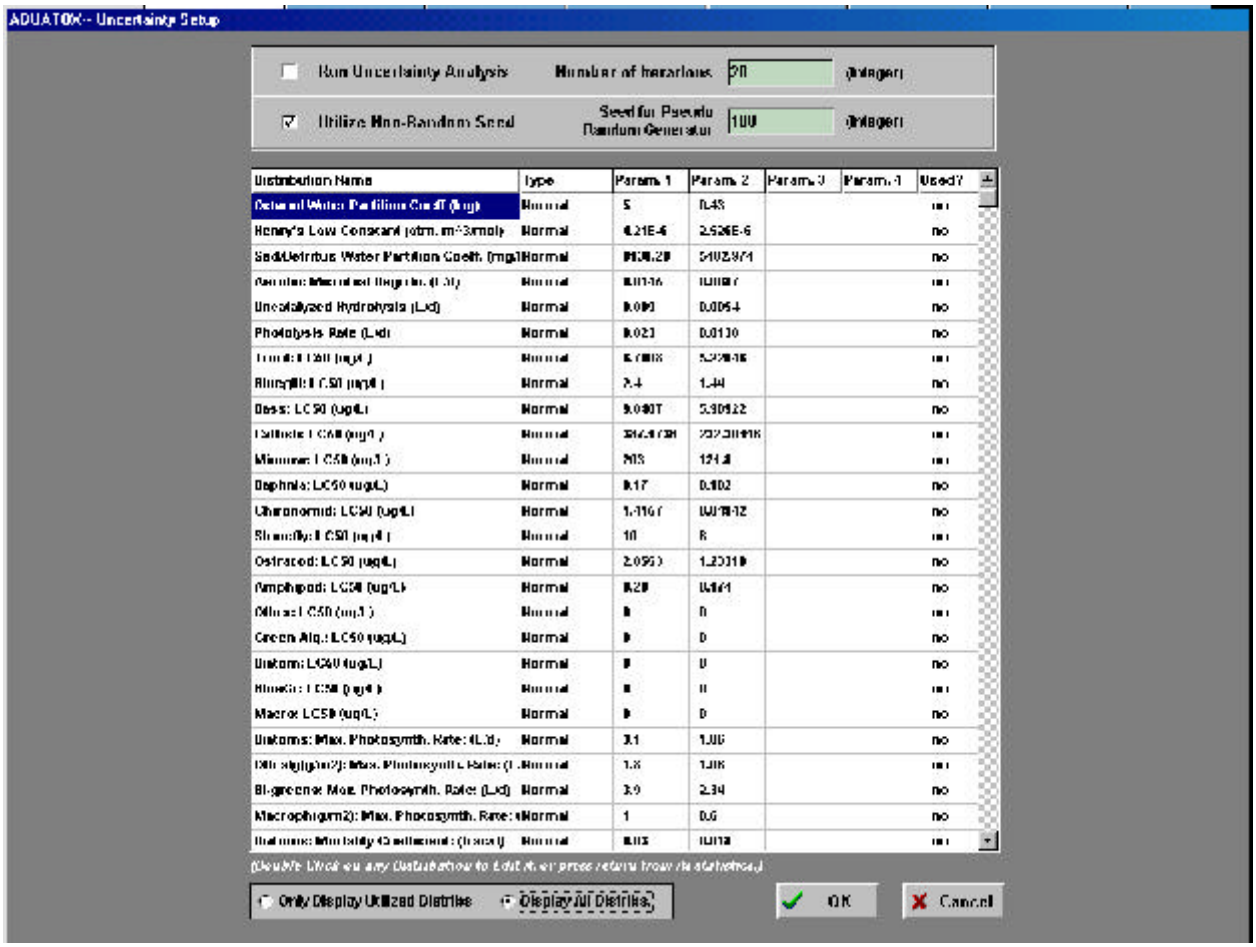
In conclusion, AQUATOX can be used to analyze complex relationships in impaired ecosystems and to suggest the relative importance of various causes of impairment. In this example, dieldrin was shown to be a very important stressor. The simulations suggest that external loadings of nutrients and organic matter are far less important; and, based on the model, halving the loadings might not improve water quality significantly but might decrease the productivity of sport fish. Therefore, this ecosystem model has the potential not only to help identify stressors, but to assess possible environmental management scenarios as well.

4. UNCERTAINTY ANALYSIS

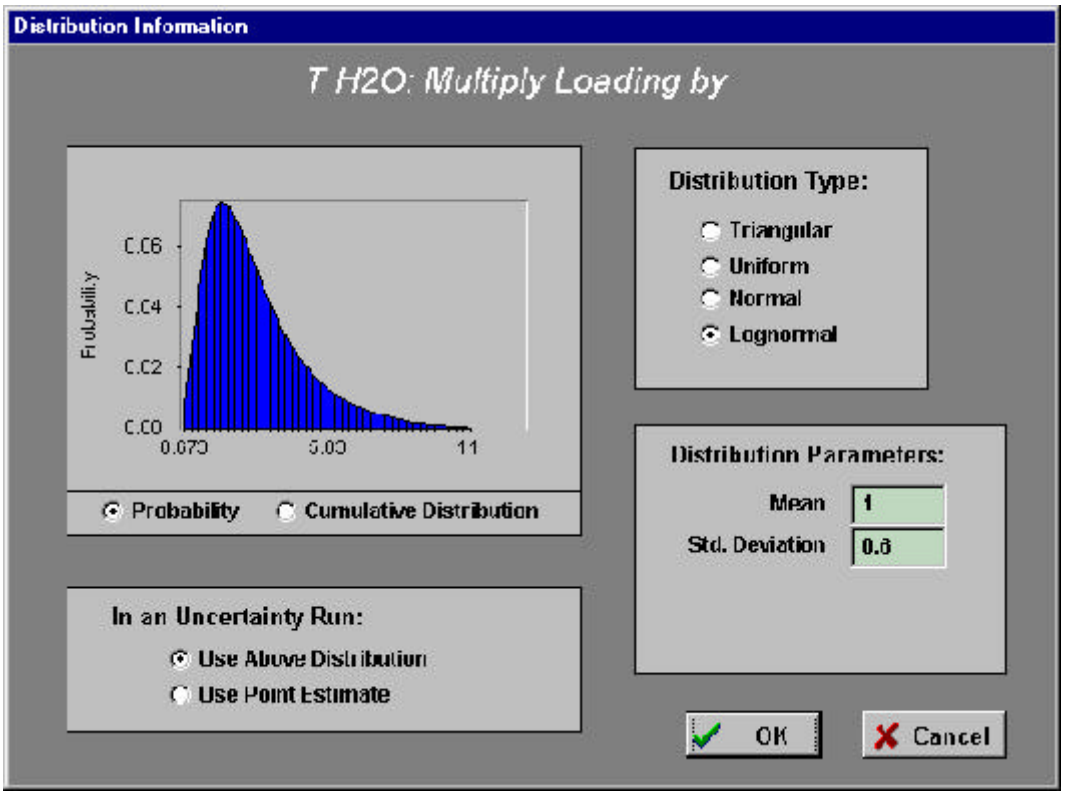
Until now we have dealt with deterministic simulations. However, there are numerous sources of uncertainty and variability in natural and polluted aquatic systems. These can be represented easily in AQUATOX (see **Volume 2: Technical Documentation**), although access to the additional analytical power is not obvious to the casual user. The key is to click on the **Setup** button and choose **Uncertainty Setup**. We will go back to the ESFenPond study for this example.



That will open a window that lists either all variables subject to uncertainty analysis or those variables already chosen for analysis. We will display all variables. Because AQUATOX uses a Latin hypercube sampling algorithm, it requires far fewer iterations than a brute-force Monte Carlo sampling. Therefore, the default number of iterations is 20. This is probably adequate for an analysis involving a single variable; however, it should be increased as more variables are chosen for analysis. If you wish to replicate the sampled values in successive analyses, you should choose a non-random seed for the number generator and keep it the same.

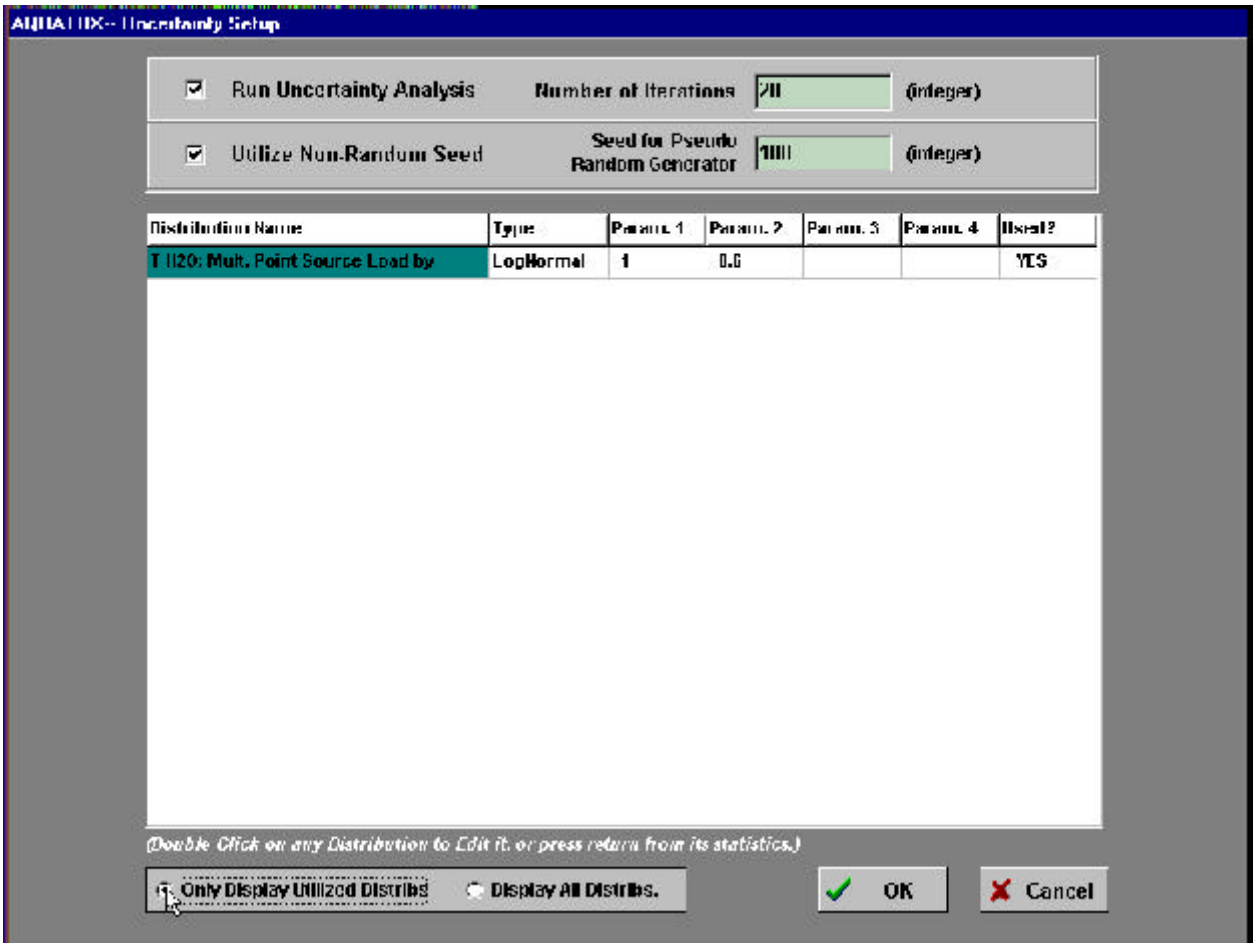


By double-clicking on a variable the distribution can be displayed and edited. The lognormal distribution is the default for loadings. The user can accept the default distribution parameters or change them. The graph will show the results of any changes. The mean values are derived from the underlying parameter sets, but altering them in the uncertainty screen will not change them in the database and the deterministic simulation.

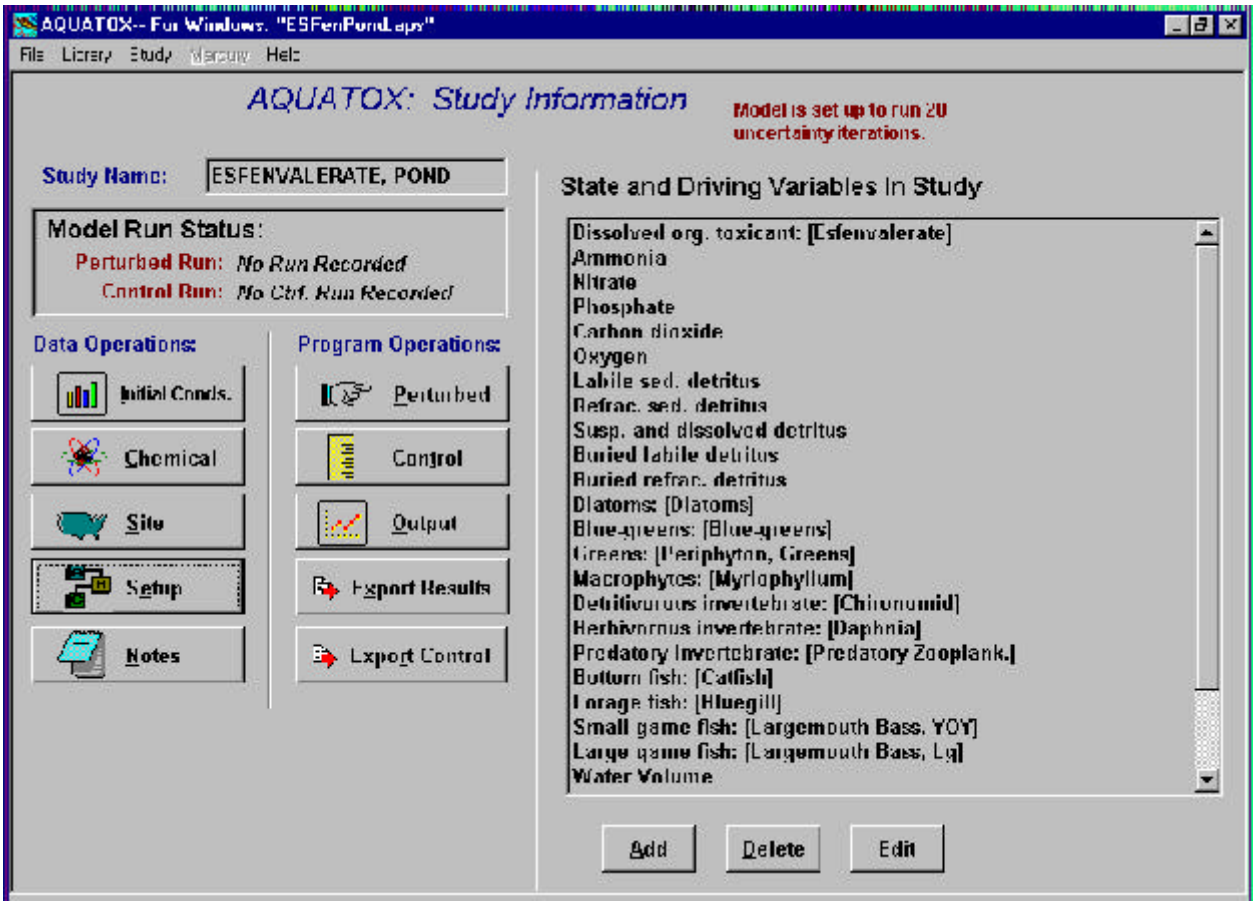


Let's use that distribution to vary the multiplicative factor for point-source loadings of esfenvalerate in water. For each iterative simulation the model will sample one value from the distribution and use it as a multiplicative factor for all dynamic point-source loading values.

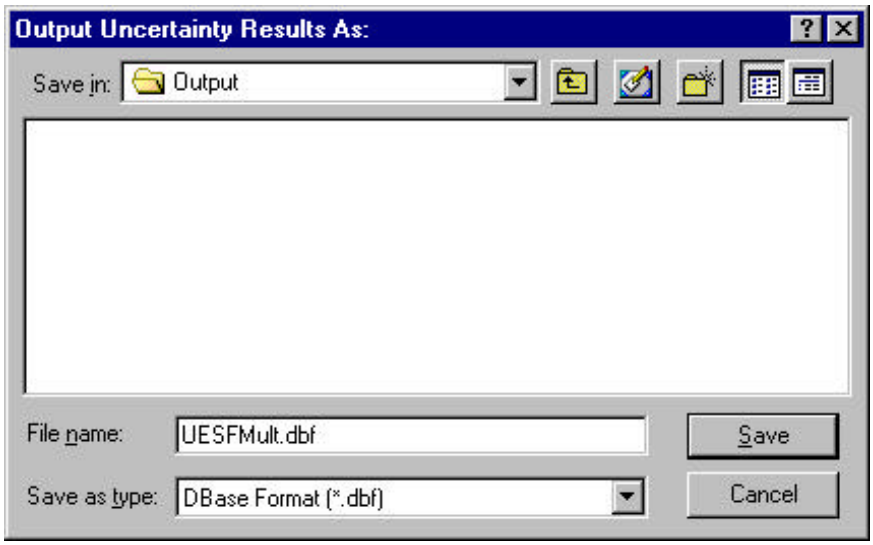
Click on **OK**, which will take you back to the list of variables; then choose to display only those that will be varied in the uncertainty analysis. Be sure that the button in the upper left is checked to **Run Uncertainty Analysis** (that button is a convenient way to toggle between the deterministic and uncertainty options without disturbing the individual distributions).



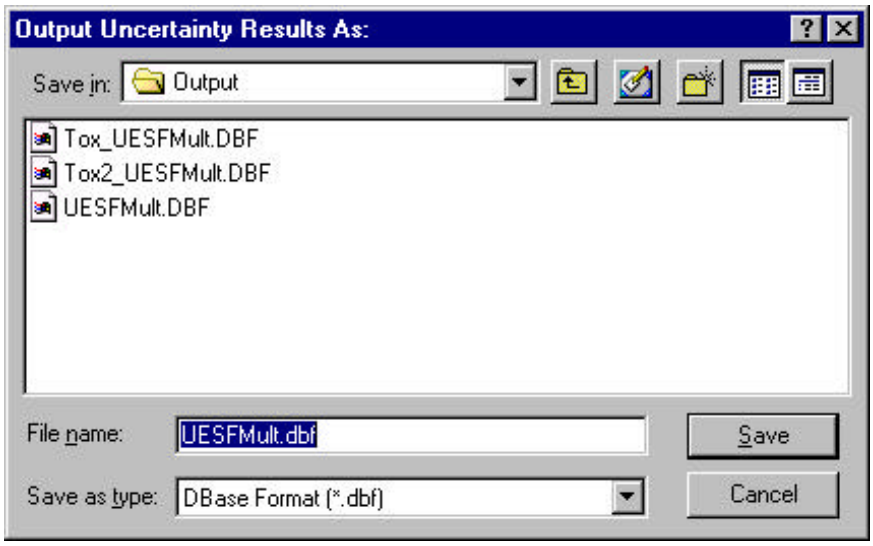
Close the **Study Setup** screen by clicking on **OK.** Back on the main screen we see that there is now a message in red in the upper right indicating the number of iterations chosen. That message only appears when the uncertainty analysis is enabled.



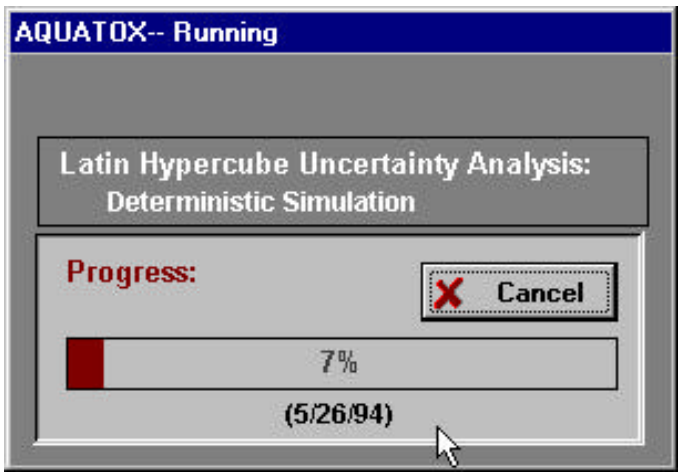
When you click on **Perturbed** or **Control** you will be asked to give the output file name and location. The folder to **Save in** will be given as the Studies folder, which is active; you might wish to change that to the Output folder. Be sure to specify the extension "dbf" or you will get an error message.



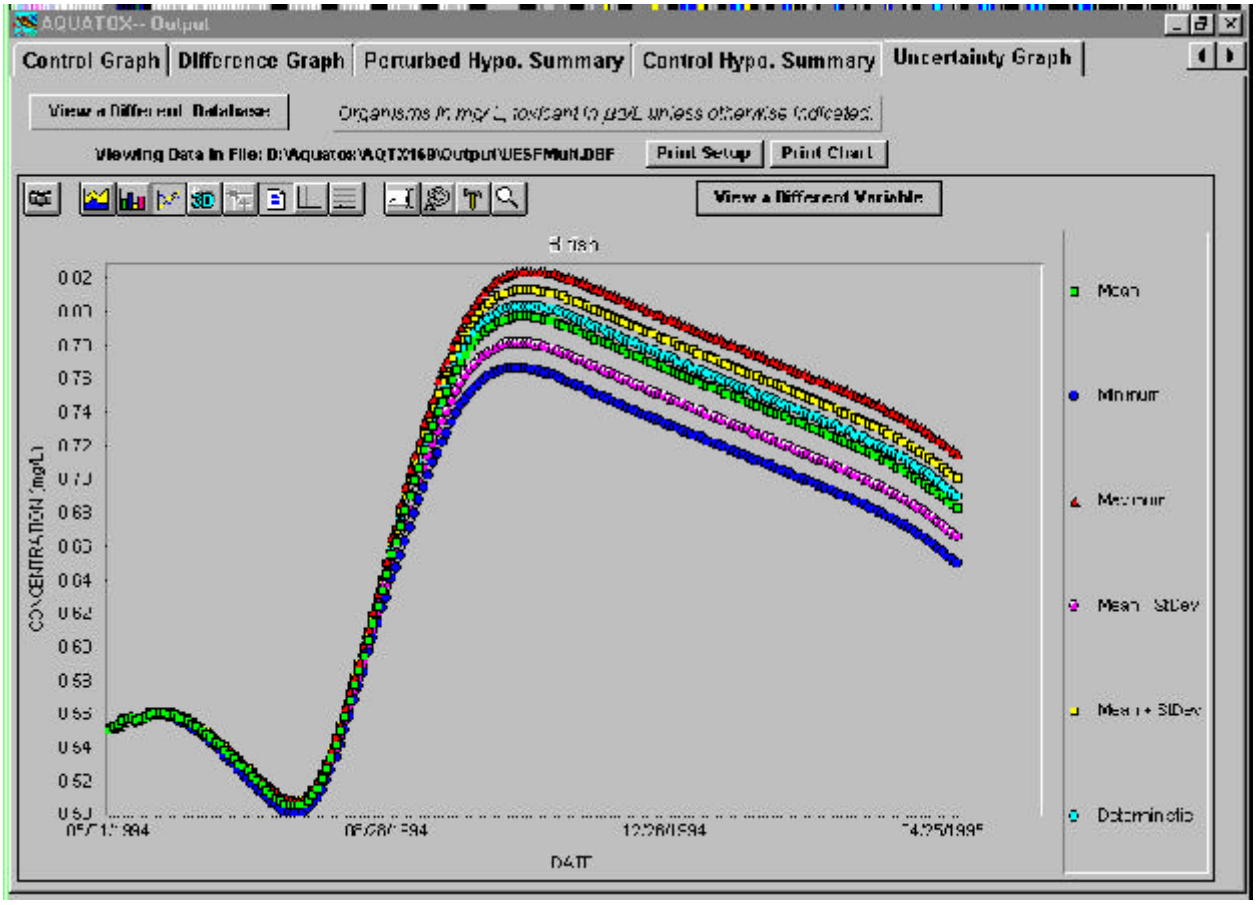
Because of the voluminous output, it will be split into three separate files using the root name that you provide. Ordinarily, you will not have to concern yourself with the supplemental files., which will be listed in subsequent Save operations.

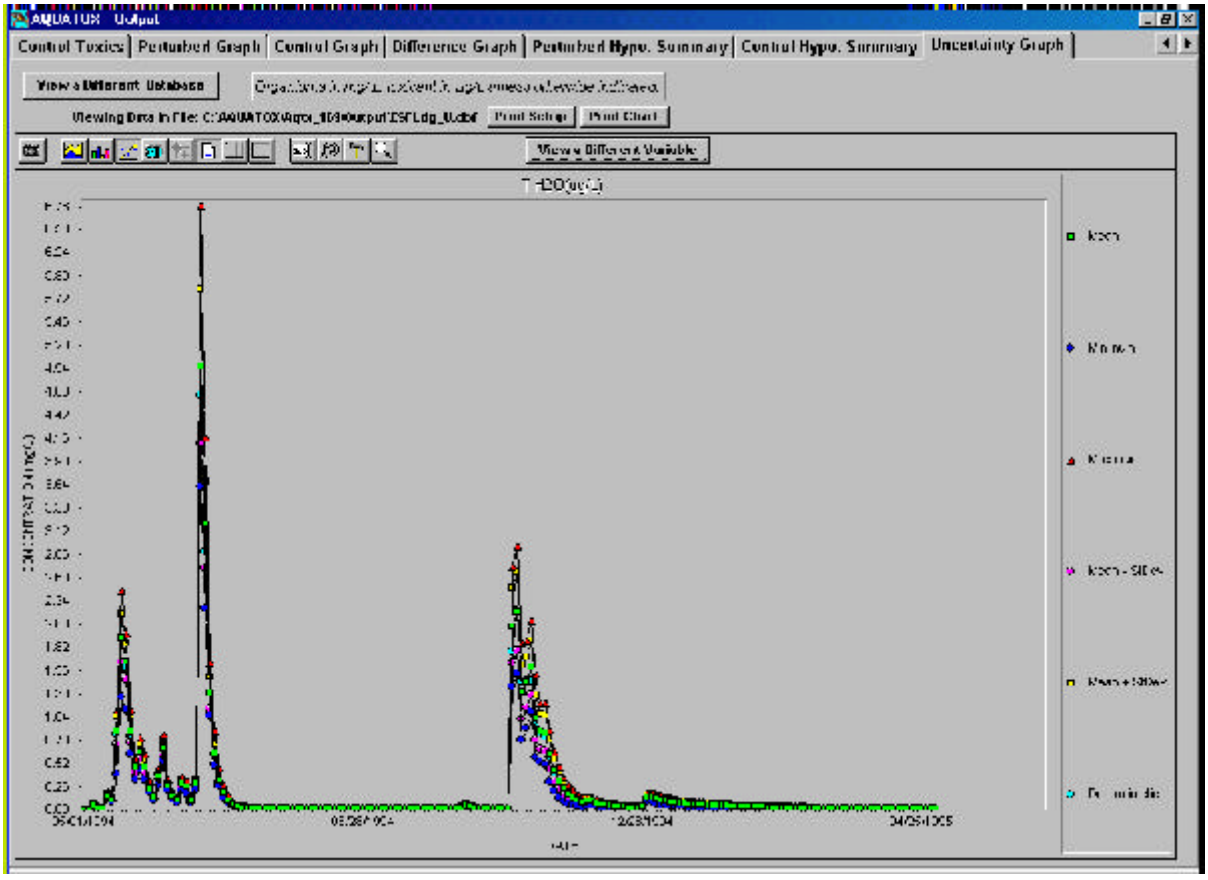


The model will perform a deterministic simulation first to provide a baseline. Then it will cycle through the uncertainty iterations.

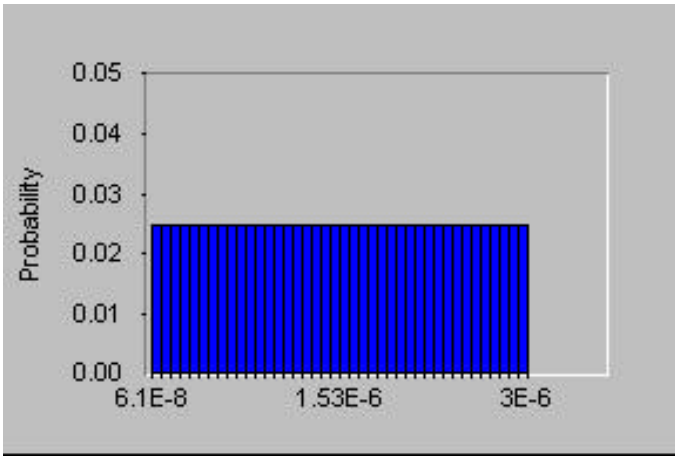


The results of the uncertainty analysis can be viewed by scrolling to the far right tab in the **Output** on the main screen, and clicking on **Uncertainty Graph**. (If you have not run a simulation or if you wish to see the results of a different simulation, you may choose to **View a Different Database**.) Only one state variable is plotted at a time, with separate curves for mean, minimum, maximum, mean - one standard deviation, mean + one standard deviation, and deterministic results. These are the distributions of the results for that particular state variable and are not necessarily a reflection of the distribution of the sampled input variable. For example, the maximum loading of esfenvalerate would almost certainly result in the minimum biomass of the large game fish, but the benthic fish that is graphed is most likely responding to decreased predation. You may choose to **View a Different Variable**, such as the concentration of the toxicant in the dissolved state. The default Y-axis label assumes that you are plotting biomass, so it should be changed to units of "µg/L" if you plot toxicant concentration.

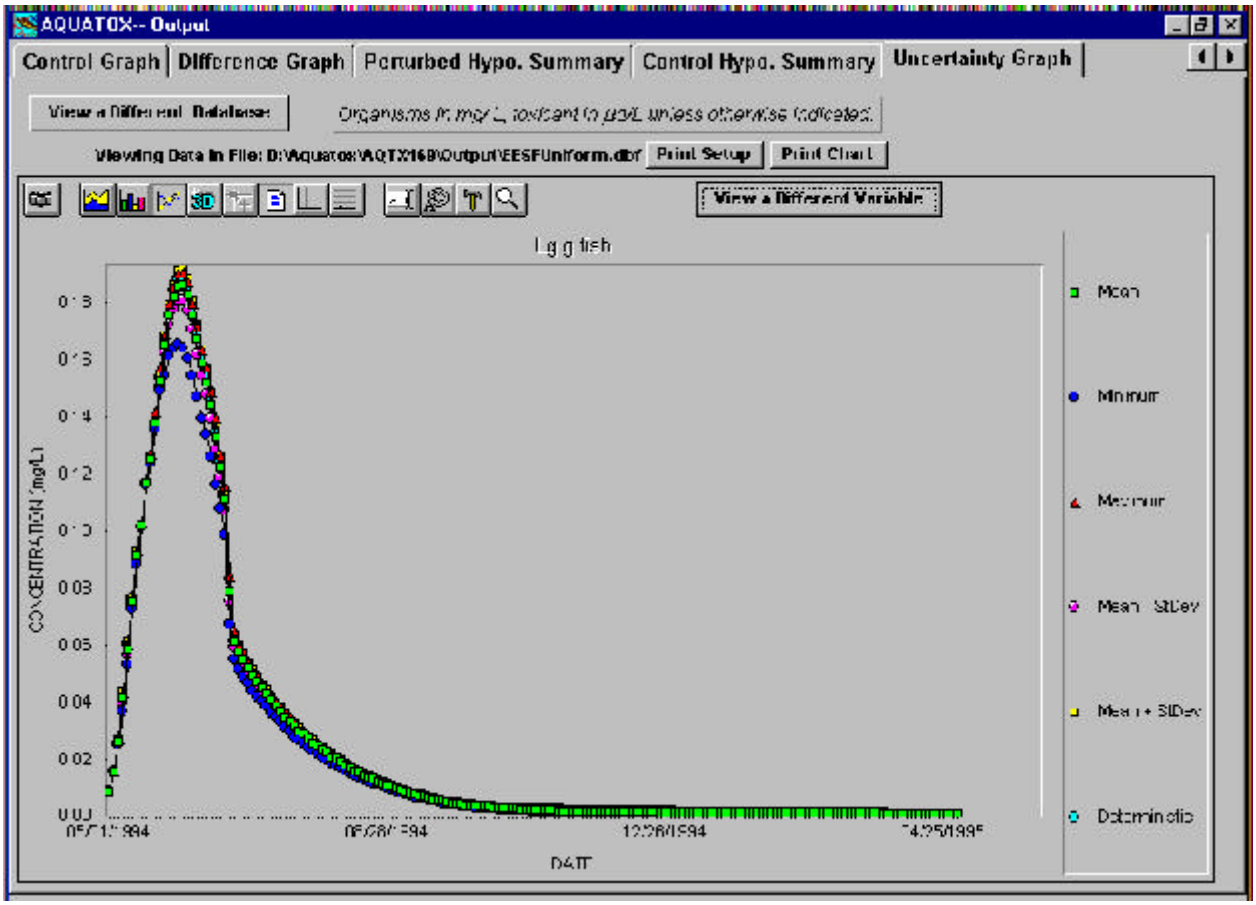

AQUATOX-- Output
Control Graph
Difference Graph
Perturbed Hypo. Summary
Control Hypo. Summary
Uncertainty Graph
View a Different Database
Organisms in mg/L, toxicant in µg/L unless otherwise indicated.
Viewing Data in File: D:\Aquatox\AQTX2i6B\Output\UESFMuN.DBF
Print Setup
Print Chart
View a Different Variable
Mean
Minimum
Maximum
Mean StDev
Mean + StDev
Deterministic
DATE



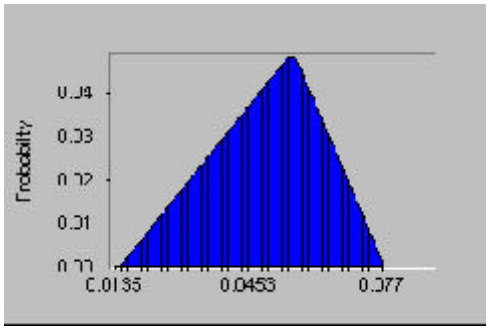
Similarly, we can vary the input values for other variables by sampling from the appropriate distributions. For example, we have two values for the Henry's Law constant for esfenvalerate: a measured value of 6.1E-8 and a calculated value of 3.0E-6 (ARS Pesticide Property Database). Why not just use the measured value? Unfortunately, the constant is not easily measured, so the calculated value may have as much validity as the measured value. Therefore, we can use a uniform distribution defined by the two values, with equal probability of any value over that range being chosen. Henry's Law constant helps control the bioavailability of organic toxicants, so the sensitivity to a range of possible values is of interest.



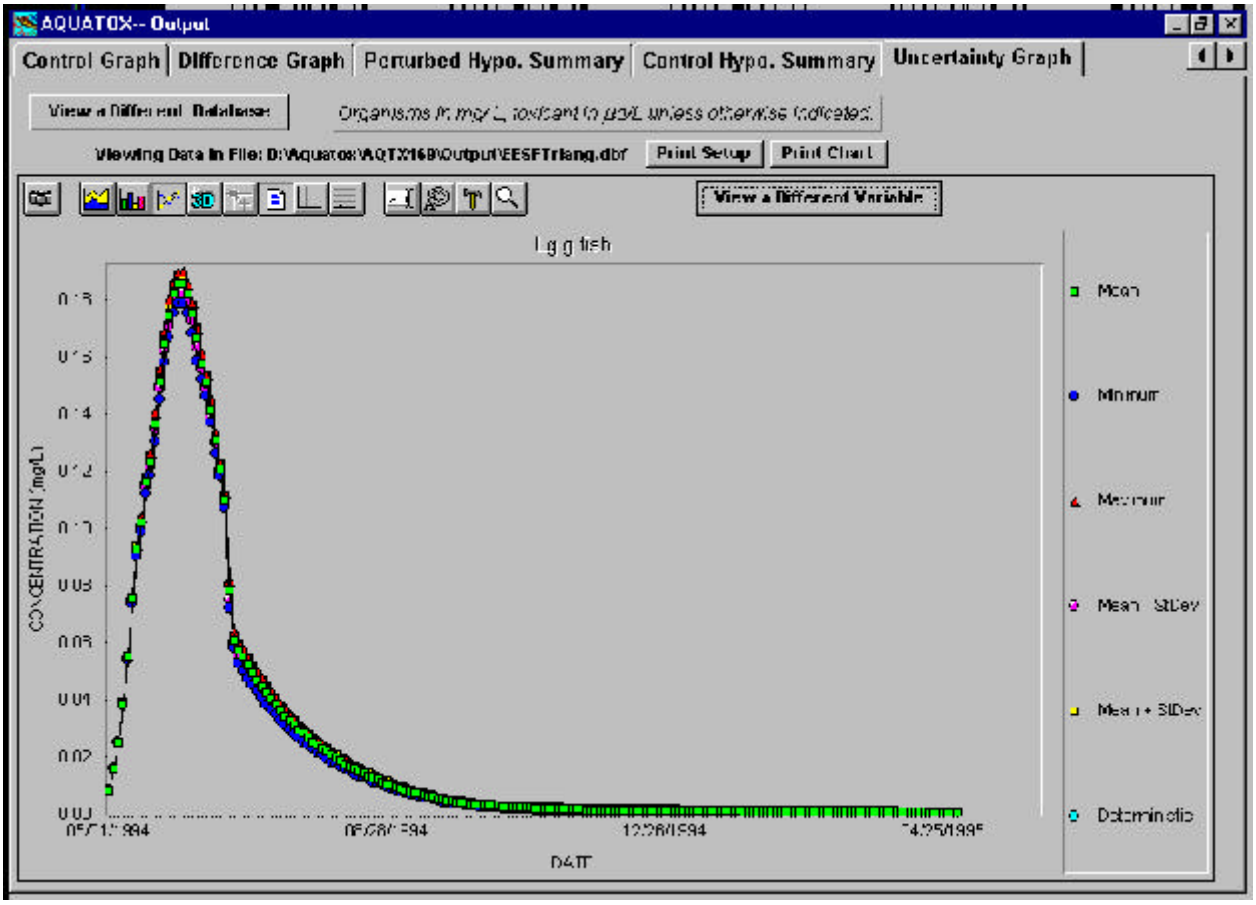
The results of varying just the Henry's Law constant for esfenvalerate are shown in the Uncertainty Graph for large game fish biomass. The spread of values, although not appreciable, is due to the differences in bioavailability and therefore differences in amount of toxicity.



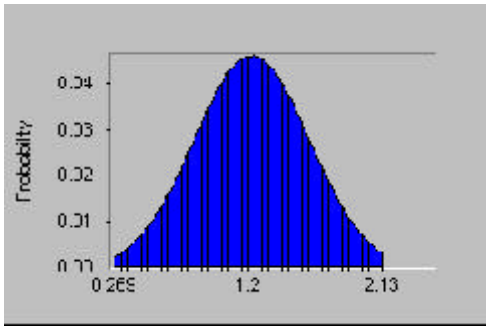
In another example, we will vary a critical parameter for the large game fish, bass, to see how it affects the response of this important species. The most likely maximum consumption rate is set at 0.055 g/g-d based on application of an allometric equation that relates consumption to mean weight (Hewett and Johnson, 1992); however, there is considerable variation reported in the literature (Leidy and Jenkins, 1977). The extreme values reported are 0.015 and 0.07. We could take these as the constraints for a triangular distribution, but that would mean throwing out the lowest and highest observed values because the constraints have zero probability. Therefore, we will extend the constraints by 10% of the observed values.



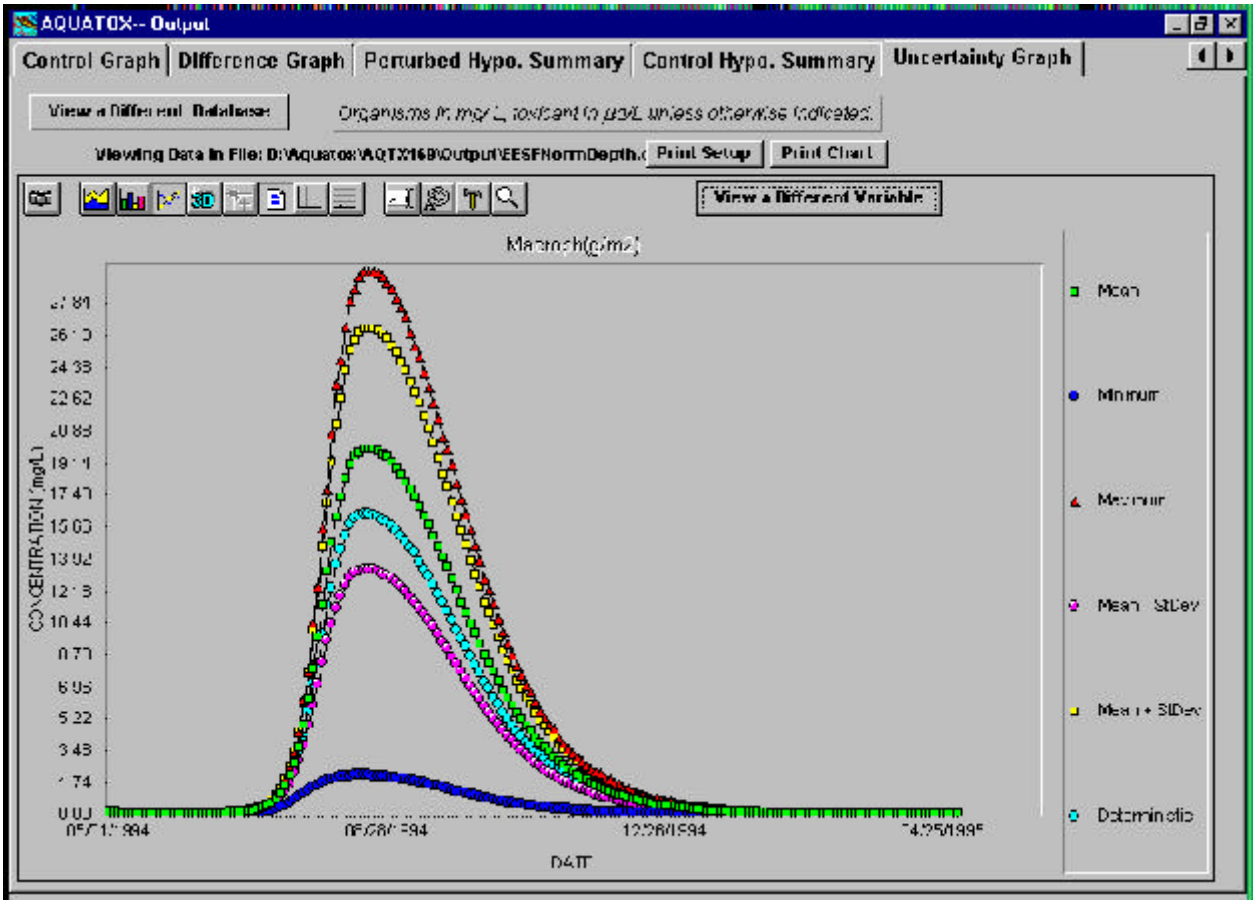
The results of varying this one parameter indicate that the model is not sensitive to it—probably because the chronic and acute toxic effects dominate the simulation.



In the final analysis we will examine the effects of varying mean depth of water in the pond. A normal distribution is used with a mean of 1.2 m and a standard deviation of 0.4. The minimum depth simulated was 0.097 m, and the maximum depth was 1.86 m.



The macrophyte biomass is sensitive to water depth. As rooted vegetation, macrophytes are well adapted to shallow water; the maximum biomass is at the minimum depth. However, they are probably light limited at the greater depths simulated in this turbid pond.


AQUATOX-- Output
Control Graph
Difference Graph
Perturbed Hypo. Summary
Control Hypo. Summary
Uncertainty Graph
View a Different Database
Organisms in mg/L, toxicant in µg/L unless otherwise indicated.
Viewing Data in File: D:\Aquatox\AQTX169\Output\EESFNormDepth.
Print Setup
Print Chart
View a Different Variable
Mean
Minimum
Maximum
Mean StDev
Mean + StDev
Deterministic
DATE

5. DATA CONSIDERATIONS

AQUATOX has many possible loading variables and process-level parameters. What input data are most critical for the simulations? The answer depends on the goals of the simulation and the site-specific requirements. By using the principles outlined above in **Uncertainty Analysis**, one can perform sensitivity analysis to identify the more sensitive parameters and loadings for a particular simulation. Sensitive parameters may require site-specific determination or careful calibration. Some sensitive variables were suggested in the above analyses, others have been identified in other studies.

5.1 Toxicant

- The octanol-water partition coefficient is critical to bioaccumulation in organisms and partitioning in detritus. It often can be estimated better than it can be measured.
- Henry's law constant is important for volatilization and yet is often difficult to measure.
- Chemical and microbial degradation parameters determine the persistence in an ecosystem. If only half-lives are reported, they should be represented as uncatalyzed hydrolysis rates, which are not affected by seasonal conditions as are microbial rates.
- The thickness of the active layer, represented as the mass of sediment detritus, is important because of the simplifying conceptualization in this version that treats sediment-water interaction of contaminants as very efficient but restricted to the active layer.
- Some toxicants, such as parathion, may bind more tightly to sediments than indicated by organic partitioning. Estimation of the sediment partition coefficient may need to be overridden with observed values.

5.2 Nutrients and Remineralization

- The fraction of phosphate that is available depends on the nature of the phosphate loadings. The model distinguishes between detrital loadings, with implicit phosphorus content that is more or less available depending on whether the material is refractory or labile. Phosphate loadings may be in the dissolved phase or may be bound tightly in mineral particles; the user accounts for these by varying the fractional multiplier: 1.0 if the phosphate is readily available and a small fraction if it is tightly bound.
- Release of phosphate from anaerobic sediments is a constant (during periods of anoxia) that is set in the **Remineralization** screen (available by clicking on **Site**). Site-specific values are appropriate where iron-dependent biogeochemistry processes are dominant.
- Co-precipitation of phosphate with calcium carbonate is not modeled. In sites where that is important the best work-around is probably to decrease the loading accordingly.
- Chemical oxygen demand is not modeled explicitly because of its site-specific nature; a work-around would be to decrease oxygen loadings.
- Constant stoichiometry for nutrients in organic matter is a simplifying assumption. One can change the value of the ratio of a given nutrient to organic matter in the **Remineralization** screen. The Redfield (1958) ratio is used as the default.
- The proportions of refractory and labile and dissolved and particulate organic matter in a

system control the rate of remineralization. Inappropriate initial conditions will cause a transient response, but poor characterization of loadings may affect the long-term nutrient budget and bioavailability of organic contaminants. If possible, obtain seasonal values for total organic carbon (TOC), dissolved organic carbon (DOC), and biological oxygen demand (BOD, which is labile); these can be used to obtain the necessary proportions. Otherwise, consider the source of detritus loadings (forests, treatment plant, etc.) when deciding how much may be refractory and particulate.

5.3 Plants

- Half-saturation constants for nutrients control how responsive phytoplankton and periphyton are to eutrophication; parameter values may depend on trophic status.
- Maximum photosynthetic rates determine the competitiveness and resilience of algae; observed rates vary greatly and composite rates, such as for a diatom community, are most appropriate for most applications.
- The model assumes that blue-green algae (or any alga occupying that compartmental slot, such as cryptomonads in the Onondaga Lake example above) float unless the wind exceeds 3 m/s; this makes the model sensitive to the mean wind loading.
- Most macrophytes are sensitive to fall dieback; cold-tolerant groups, such as charaphytes, should be so characterized with appropriately low optimal temperatures.

5.4 Animals

- Consumption of refractory detrital sediments by zoobenthos increases the degradation rates of those sediments, increasing the simulated sediment oxygen demand and remineralization. The user should assume that most zoobenthos selectively feed on labile detritus, which includes freshly sedimented algae.
- The minimum biomass for feeding (Bmin) is seldom measured, yet the model can be very sensitive to this. The BMin value protects prey from being totally consumed, but if it is set too high the predators may starve to death. It may require site calibration.
- Half-saturation for feeding is very seldom measured, but it can significantly reduce predicted feeding rates. Therefore, it should be set low in the absence of data.
- Consumption and respiration rates in fish are functions of body size. Most default values are based on application of allometric equations presented by Hewett and Johnson (1992). Selection of representative mean weights for use in the equations is important.
- Mortality rates may vary greatly from one site to another. This often becomes a calibration parameter, especially since death due to predation is separate in the model.
- If modeling an aquatic insect that emerges, be sure to select "Benthic Insect" in the drop-down list in the parameter screen because otherwise emergence will not be simulated.

5.5 Inorganic Sediments

- Inorganic sediments are not explicitly modeled for standing water and only roughly for streams. This simplification reflects the model's emphasis on nutrients and organic

contaminants. If sediment transport, burial, and scour are important, the model should be coupled to a hydrodynamic model such as EFDC.

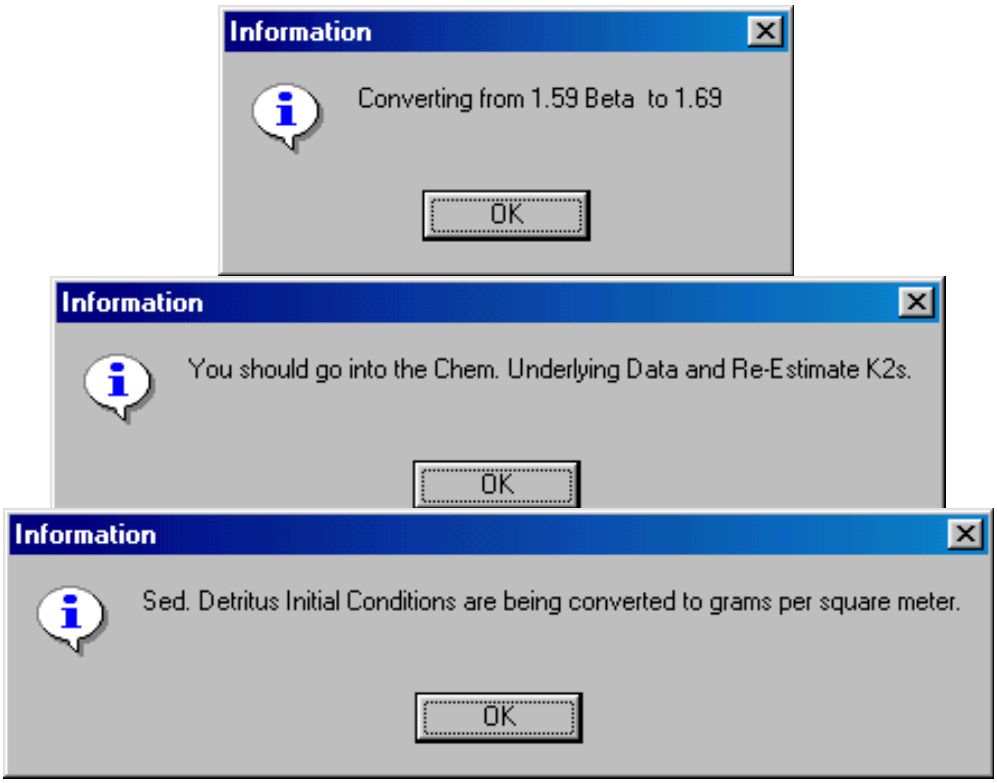
- Total suspended solids are used to back-calculate suspended silts and clays in the model. Because this is a loading that is compared with phytoplankton biomass in the computation of Secchi depth and light extinction, it should be provided for the entire period of the simulation (most loadings can be repeated automatically if the simulation period is longer than the available data).

6. QUALITY ASSURANCE

AQUATOX is designed to facilitate documentation of assumptions and data sources for specific applications and to archive results. Note fields are provided for the study and for each of the state-variable loading screens. These are intended to provide the user with a way to record an overview of the study and to describe sources and salient features of the loading data. Furthermore, almost every parameter has an associated comment field to document the source of the value used. These fields are not fully utilized in the example sets; but, as additional data are incorporated, comments should be used liberally.

A study, with all associated data and output, can be archived in a study file. *Good practice dictates that the version of AQUATOX used for the application should be saved as well.* In that way the study can be opened and results examined at any time; and, if necessary, the model can be re-run. The main screen indicates the dates and times that the perturbed and control simulations were run, but be careful: opening some screens, such as **Setup**, will reset the status to "Run Not Current." If you make a change to a study, you may choose not to save the changed file. To minimize file size, do not save the output; this can be done by clicking on **Study** on the menu bar in the main screen and choosing **Clear Results**. The file will usually be much smaller, but you will have to re-run the simulation to see the results.

AQUATOX versions are upward compatible within reason—but not necessarily years later—so if you open an old study with a newer version of the model, the data structure will be updated. Usually this is automatic, but sometimes the user may be directed to assist in the upgrade, as shown in the sequence of information windows below.



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Park, R.A. 1999b. *Validation of the AQUATOX Model, Version 1.66, with Data from Lake Onondaga, New York.* In: AQUATOX for Windows: A Modular Fate and Effects Model for Aquatic Ecosystems–Volume 3: Model Validation Reports. U.S. Environmental Protection Agency 2000. EPA-823-R-00-008.

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